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THE CLEAVAGE SURFACES OF GALENA[1]

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In general, the microscopic study of the sulphide minerals has been confined to the examination of surfaces that have been developed by grinding and polishing. The surfaces thus produced differ materially in some respects from those resulting from natural breakage or crushing, since they are the result of surface flowage and may therefore be considered as representing artificial surfaces.

This paper deals with the physical and structural characteristics of natural galena surfaces resulting from chipping or breaking pieces approximately one-half inch in diameter from large specimens and examining them by means of the reflecting microscope.

The samples studied were collected from a variety of sources but originated chiefly in the Joplin district, Missouri. They consisted of several types of the coarse crystalline galena, and the specimens varied in size from fairly uniform cubes approximately one inch in diameter to specimens up to ten inches in diameter.

The procedure followed was to chip off a fragment of galena with a sharp chisel in order to avoid extensive internal fracturing and at the same time procure a specimen having a surface approaching a plane. The specimens were then cleaved to approximately $\frac{1}{2}$-inch size for study with the reflecting microscope. Smaller pieces, of sizes down to +200 mesh, were also examined and were prepared for study by mounting them in a plastic clay.

Cleavage faces of galena are remarkable for their luster, which far surpasses that ordinarily attained on surfaces that have been prepared for microscopic study by grinding and polishing. When seen through the microscope, natural cleavage faces show many outstanding and interesting characteristics which may be of value to the metallurgist from the standpoint of ore treatment and are also worthy of consideration in the study of crystal structure.

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The galena specimen shown in Figure 1 illustrates the popular conception of "a perfect cube" which may be taken to mean that its form closely approaches that of the conventional illustration used in textbooks on mineralogy and crystallography. Presumably, such a cube may be considered by many to represent a unit or individual cube because examination of its surface shows no evidence to the contrary. Several specimens of this type, all from the Joplin district, were examined. All were smooth and no conception of their internal structure could be gained from surface observation. However, when the outer surface was removed by chipping with a chisel, it was apparent that such cube specimens were made up of innumerable smaller individual cubes.

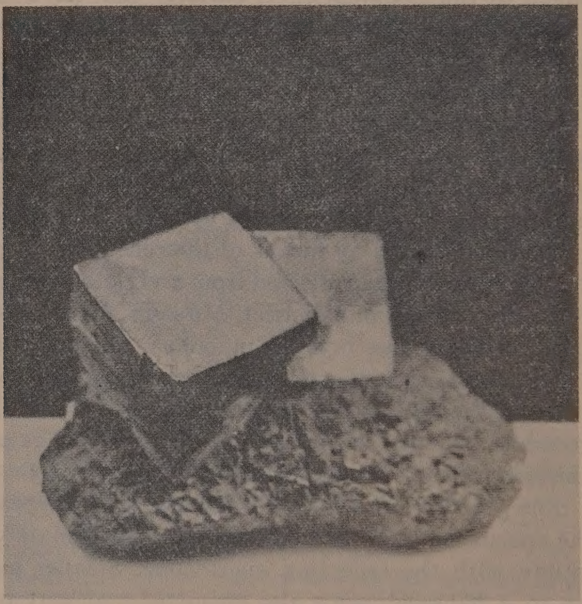

FIG. 1. Symmetrical cube of galena from the Joplin, Missouri district. Approximately natural size. These cubes show no surface indication that they are made up of innumerable, associated blocks or cubes of galena.

Examination of the freshly cleaved surface by reflected light disclosed a variety of interesting surface characteristics. Some areas were apparently perfectly flat, highly reflective surfaces, free from pits or imperfections. In other cases, surfaces showed a well-defined "checkerboard" pattern of lines crossing each other at 90°

angles, obviously outlining the cleavage planes and marking the characteristic cubes which result when galena is subjected to crushing. If the visible striations on cleaved faces of galena are taken as a measure of the size of the component blocks, it is evident that these units are of extremely small size. In examining the finest sets of striation lines observed with an oil immersion objective at a magnification of 750 diameters the distance between lines was found to lie in a range from 0.005 mm. to 0.001 mm. (5 microns to 1 micron). Whether or not these dimensions may be taken as that of the smallest unit cube is not certain. It is certain, however, that galena will break into cubes of the dimensions indicated. It is of interest to point out that the striations under discussion are in reality a manifestation of surface irregularities. As a matter of fact, it is due to the existence of surface irregularities that the striations are rendered visible. There are areas in which the preceding characteristics are well defined but in addition show another set of lines not so strongly marked, but

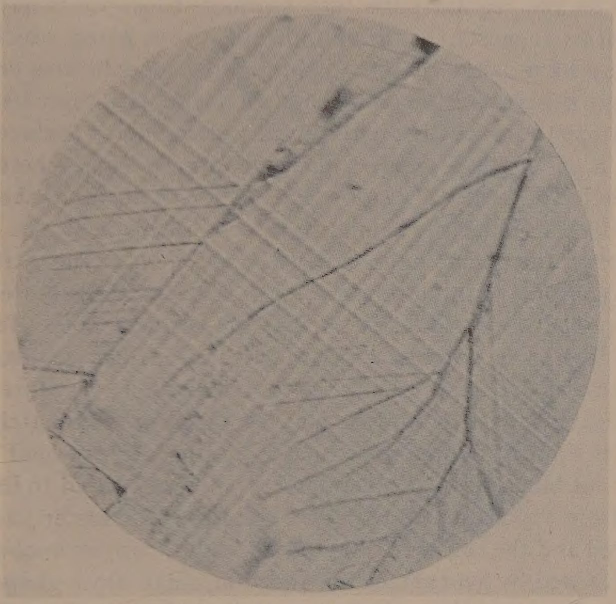

FIG. 2. (Magnification 400×). Shows "lattice structure" or outlines of cubic cleavage, also tree-like, surface indications of "slip planes," which in some cases are open and whose surfaces may be etched and non-reflective or smooth as in slickensides.

clearly visible, extending diagonally across the cleavage lines at an angle of approximately 45°.

When viewed in reflected light, especially with the higher power objectives, the striated surfaces described exhibit surface characteristics strikingly similar to linen or other like material when viewed through a magnifier, *i.e.*, they are suggestive of a mesh-like or woven surface.

Reference to Figure 2 shows, in addition to the block cleavage, two sets of irregular, tree-like striations that are equally as well marked as the regular cube face outlines. Close examination of these forms suggests that they indicate planes along which slippage may have taken place and through which solutions or gases may have penetrated the cube mass. In some cases these channels are still open and when exposed by dissection show surfaces that present a pebbly appearance indicative of corrosion. Where these channels have "healed," *i.e.*, been filled in or cemented, they present surface irregularities similar to those of the cube blocks.

Although the galena cube under discussion was symmetrical in surface contour, examination of its interior structure showed that its component blocks did not parallel the surface planes. This deviation was more pronounced with increase in distance from the outer faces of the cube and amounted to a distinct curvature in the block arrangement. One of the cleaved faces, approximately one-half inch square, showed a distinct radiating arrangement of the component blocks from a central point which appeared to have resulted from exposure to a corrosive solution. The luster had been destroyed and the surface presented a "pebbly" appearance similar to that caused by acid attack. In addition, small block-shaped pits had been developed through the removal of cubes of galena. This removal had taken place along roughly symmetrical lines which gave the impression of a radiating structure on the surface affected. Crystals of lead carbonate had developed in several places on the corroded surface, undoubtedly formed by the decomposition of the galena. In general, the lead carbonate crystals were distinctly visible under a binocular microscope at a magnification of 5 diameters.

The occurrence of lead carbonate and lead sulphate associated with galena is common, but the presence of lead carbonate within a galena cube would not be expected.

Crystals of sodium chloride were commonly found oriented along striations on the galena surface (see Fig. 3). They ranged in size from 0.026 to 0.001 mm. The axes of the halite crystals generally paralleled the visible galena cubic structure, even when occurring along diagonal striations. This occurrence was observed in all specimens examined from the Tri-State district and leads to the belief that sodium chloride is a natural and common constituent of the galena in that region. In addition to whatever significance the occurrence of halite with galena may have from mineralogical and ore-dressing standpoint, it has a geologic interest worthy of mention, namely, the origin of the ore bodies of the Joplin, Missouri, district. This matter is discussed in detail by H. F. Bain,[3] and is briefly summarized by Waldemar Lindgren.[4] A theory advanced concerning the origin of the lead deposits of southeastern Missouri involves the transportation of the lead into the Cambrian sea by

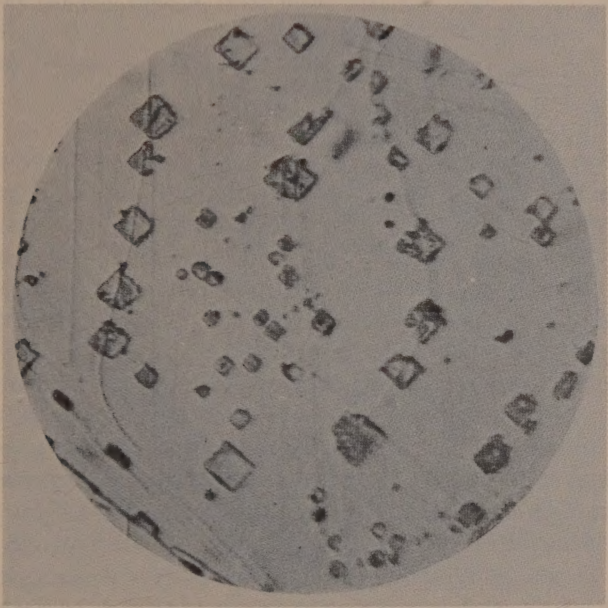

FIG. 3. Crystals of sodium chloride (halite) on natural cleavage face of galena from the Joplin district, Mo. The salt crystals range in size from 0.02 mm. to 0.001 mm. and appear to be a natural constituent of the coarsely crystalline galena from the Joplin region.

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[3] *Bull. U.S.G.S.*, No. **294**; Zinc and Lead Deposits of the Upper Mississippi Valley (1906).

[4] *Mineral Deposits*. McGraw-Hill Book Co., *New York*, **1919**, See pages 461–464.

flowing tributary streams, deposition with the Bonneterre dolomite, followed by concentration by surface waters after the subsequent formations were laid down.

Although the foregoing surface and structural features are described as existing in the symmetrical galena cube specimens, they are possessed in common by all the coarsely crystalline galena specimens from the Joplin district that were studied. In addition to the conditions described, other structural characteristics appear to be common to these coarsely crystalline varieties of galena.

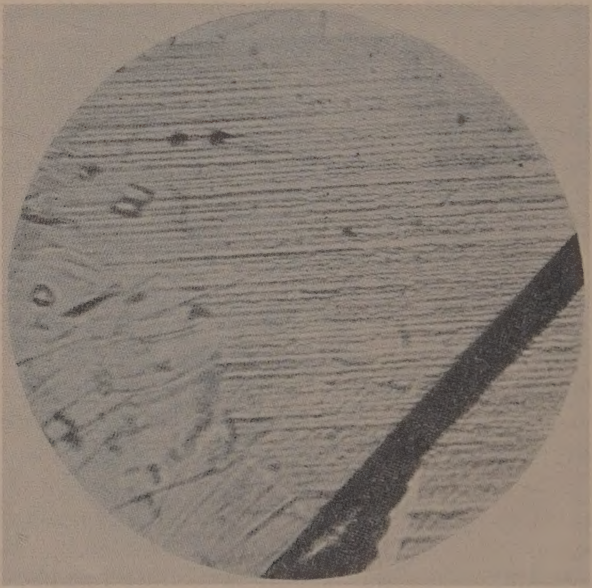

FIG. 4. Parallel striations extending across a natural cleavage face of galena at an angle of approximately 45° to the cubic cleavage. Magnification 225×. The distance between the lines shown is approximately 0.004 mm.

In examining numerous cleaved faces of galena specimens, many slip planes were observed which undoubtedly indicate a condition of stress and strain within the mass. By dissection methods, material was removed along several of these planes. Two distinctly different types of surface were found to exist. In some instances the surfaces were smooth and highly reflective, approaching the condition of block cleavage surfaces. In others the surface of the slip plane was dull and lusterless and had the appearance of having been etched or corroded.

These two types of slip surfaces are probably the same, the differences in surface characteristics being due in the one case to the penetration and circulation of gas or solutions which attacked and destroyed the reflective surface, and in the other case to the absence of such a condition.

Voids are quite common in masses of galena made up of aggregates of blocks. These voids are usually irregular in shape and vary greatly in size. In some cases they are visible to the unaided eye, (1 mm. or more in diameter) but in others they are of microscopic size. Like the slip planes, their walls may be either reflective or dull (etched), probably due to the action of the same agencies—namely, corrosion by gas or solutions or their absence.

SUMMARY

Perfect unit cubes of galena of any material size, *i.e.*, one-fourth inch, one-half inch or greater in dimensions, probably do not exist in nature. Such specimens as are found that appear to be homogeneous units are made up of a multiplicity of smaller units.

The existence of halite on galena surfaces is a matter that affords some grounds for amplification, at least theoretically. The mere fact of its presence is suggestive and might serve for entertaining the premise of the possible occurrence of other soluble or insoluble salts as natural surface constituents on sulphide minerals. Sodium chloride appears to be of common occurrence in certain galena samples from Missouri and it is not at all unlikely that further detailed study of galena and associated sulphide minerals from other mining districts may result in the finding and identification of salts of other elements such as calcium, magnesium, iron, etc.

The present study of galena, though incomplete, shows that galena possesses a variety of physical characteristics which may play some part in accounting for differences in the action of this mineral under variable flotation conditions and for differences between specimens from different localities.

KRAUSITE, A NEW SULFATE FROM CALIFORNIA

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INTRODUCTION

During a field study of the boron deposits of California and Nevada in 1929 there was found in the colemanite district of Borate, in the Calico Hills, San Bernardino County, California, a small deposit of sulfates of iron. This deposit was found to contain a fair abundance of a new sulfate of iron and potash not previously described. Earlier, in 1926, there was collected from the dumps of the Santa Maria mine, at Velardena, Durango, Mexico, a small amount of similar material which proves to be the same mineral. For this new mineral species the writer proposes the name *krausite,* in honor of Doctor Edward Henry Kraus, professor of crystallography and mineralogy and director of the Mineralogical Laboratory, University of Michigan.

LOCALITY AND OCCURRENCE

The borax camp of Borate is situated six miles from the town of Yermo from which it is readily accessible by road. The camp has long since been abandoned and is now largely fallen into ruin. The road from Yermo follows the main Los Angeles-Salt Lake City Highway for a short distance, circles the eastern end of the Calico Hills and approaches Borate by way of a dry and sandy wash. The old road to Borate continued up this wash to a small side canyon from the southwest that led directly to the old camp but this is now washed out and the newer road swings south to an old railroad grade which it uses to the camp. At the point where the old road leaves the main wash is a prominent outcrop of dark banded cherts at the southern exposure of which is a small prospect hole containing the sulfate minerals. This body of salts was known to the borax miners and was generally referred to as the "sulfur" prospect, a fair abundance of yellow copiapite being mistaken for sulfur.

The rocks in the immediate vicinity of Borate are sedimentary, sandstones, shales, marls, fresh water algal limestones and related rocks resting upon a basement of rhyolite and capped unconformably by andesite tuffs, the "calico rock" of the old silver miners of the silver camp of Calico, a few miles to the west. Near the upper part of the exposed portion of the sedimentary beds is found the colemanite that produced the borax ore mined some years ago. The sulfate bearing cherts are several hundred feet stratigraphically below this but have no apparent connection with the borate deposits.

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The sulfate body is a lenticular mass of mixed salts, probably not over 10 feet in thicknesss and the minerals contained therein, in the order of their relative abundance are: alunite, coquimbite, roemerite, voltaite, jarosite, halotrichite, krausite, metavoltite, fibroferrite, sulfur, gypsum, anhydrite and a few others that occur sparingly and are not yet fully determined. The salts are roughly zoned; the alunite occupies the foot wall and grades into sugary white coquimbite, while the center of the deposit and the hanging wall is made up of a complex aggregate of mixed salts. Krausite is found in small part in the alunite and coquimbite but more largely and in better specimens in the transition zone between the coquimbite and the mixed salts.

Krausite occurs in several different forms. That found in the alunite forms comparatively large but rough crystals, lacks transparency and often has a pale mauve color superimposed on the yellow of the purer mineral. It occupies nests and irregular cavities in the fine clay-like alunite or coquimbite. The krausite of the transition zone is in lemon yellow crystals, often clear and with brilliant luster. These crystals, rarely exceeding two or three millimeters, line cracks and are associated with colorless or purple coquimbite, brown crystals of roemerite, black cubes of voltaite and chestnut

ANALYSIS OF KRAUSITE FROM BORATE, CALIFORNIA
William F. Foshag, analyst

	1.	2.	3.
Insoluble	0.92		
CaO	0.12	.0021	
FeO	0.24	.0033	
Fe_2O_3	24.94	.1562	26.2
K_2O	14.71	.1562	15.4
Na_2O	0.64	.0103	
SO_3	51.05	.6381	52.3
SiO_2	2.19		
H_2O	5.59	.3158	5.9
	100.40		
Sp. Gr. 2.840			

flakes of metavoltite. Rarely radiated blades of a dull yellow color are seen.

CHEMICAL PROPERTIES

For analysis clear crystals or groups of crystals were selected. A small amount of coquimbite, metavoltite, clay and an unknown hexagonal mineral contaminated the sample but in amounts aggregating less than one or two percent. The analysis and ratios derived therefrom are given above.

From these results it is quite evident that the insoluble matter, lime, ferrous oxide, silica and perhaps the soda should be deducted as extraneous matter; the remaining constituents giving, in a very satisfactory manner, the ratios: $K_2O:Fe_2O_3:SO_3:H_2O=1:1:4:2$. The mineral is therefore a normal sulfate of iron and potash of the composition $K_2SO_4\cdot Fe_2(SO_4)_3\cdot 2H_2O$, the theoretical composition of which is given in Column 3.

Krausite is insoluble in water and is only slowly decomposed; crystals left for several days in water show only a superficial film of iron hydroxide. It is slowly but completely soluble in hydrochloric acid. Before the blowpipe the mineral decrepitates strongly coloring the flame violet. The mineral first becomes opaque, then assumes a red crust and finally is reduced to a black scoriaceous mass. In the closed tube it decrepitates in part, turns first ocherous yellow, then chestnut brown and finally fuses to a dull vesicular mass. Water that is strongly acid in character is given off.

CRYSTALLOGRAPHIC PROPERTIES

Krausite is found only as crystals or aggregates of crystals and abundant satisfactory material was available for measurement. The crystals seldom reach 5 millimeters in size and these are rough and deeply striated crystals from the alunite zone. The smaller crystals are often completely developed and are bright and often flawless. Numerous crystals were examined, a large number provisionally mounted on the goniometer and 16 were finally measured. These measurements show the crystals to be monoclinic in form but of several different habits. The recognized faces are: *c*(001), *m*(110), *l*(210), *a*(100), *f*($\bar{1}$02), *d*($\bar{1}$01), *r*($\bar{2}$11) and *s*($\bar{1}$12). Not all these faces gave reflections suitable for crystallographic calculations although three, *m*, *c* and *d* gave good to excellent signals. The measurements of these faces, used in the calculations are given in the following tables.

m (110)		*c* (001)	*d* $(\bar{1}01)$
33°19′	(1)	12°24′	−43°00′
30	(1)	42	19
31	(2)	44	24
36	(3)	49	32
39	(1)	51	36
40	(2)	54	
43	(2)		Average −43°22′
45	(2)	Average 12°44′	
53	(1)		
59	(1)		
Average 33°39′			

From these measurements the following crystallographic elements have been calculated.

Linear elements	Polar elements
$a=1.5401$	$p_0=1.1419$
$c=1.7584$	$q_0=1.7101$
$\beta=102°44'$	$e=0.2204$
	$\mu=77°16'$

The measured and calculated angles for all the forms are as follows:

MEASURED AND CALCULATED ANGLES OF KRAUSITE

		Measured				Calculated			
		ϕ		ρ		ϕ		ρ	
		°	′	°	′	°	′	°	′
c	(001)	90	00	12	44	90	00	12	44
a	(100)	90	00	90	00	90	00	90	00
l	(210)	52	59	90	00	53	50	90	00
m	(110)	33	39	90	00	33	39	90	00
d	$(\bar{1}01)$	90	00	−43	22	90	00	−43	21
f	$(\bar{1}02)$	90	00	−19	45	90	00	−19	45
r	$(\bar{2}11)$	−50	5	−69	43	−50	21	−69	49
s	$(\bar{1}12)$	−24	20	−43	46	−22	18	−43	24

FORMS AND HABITS

The prism *m*(110) is often the largest form on the crystals but in some habits is considerably reduced in size although it is always present. It is always sharp and bright but often slightly rounded so that it gives a multiple signal.

The orthopinacoid *a*(100) is rarely present and then only as a narrow face; a prominent cleavage in this direction often gives small reflecting surfaces.

The base $c(001)$ is always a prominent face on the crystals, sometimes occupying the entire crystal termination and usually it is the most prominent terminal face. It is always sharp giving good reflections although it is sometimes curved.

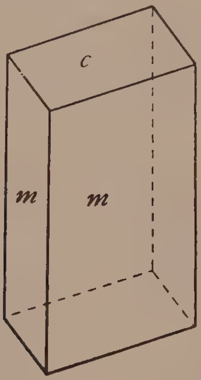

FIG. 1. Simple crystal of krausite with $c(001)$ and $m(110)$.

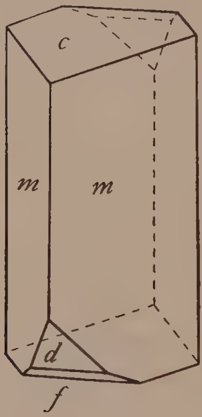

FIG. 2. Crystal of krausite with $c(001)$, $m(110)$, $d(\bar{1}01)$, and $f(\bar{1}02)$.

The two orthodomes $d(\bar{1}01)$ and $f(\bar{1}02)$ are often present but quite variable in size. The face d rarely exceeds c in size and is usually much smaller, while f is usually a small to medium sized face.

The prism $l(210)$ is rare and found only as narrow faces.

The pyramids $r(\bar{2}11)$ and $s(\bar{1}12)$ are occasionally encountered but are always much rounded, yielding poor signals. The face s is often large. Both forms appear to be solution forms.

The habit of the crystals vary from long needle-like prisms to thin, flat wedges and there are all gradations between these two extremes. The commonest habit is a medium prismatic one, terminated by the base *c* (Fig. 1), the base *c* and the orthodome *f*, or the base *c*, orthodomes *d* and *f* (Fig. 2). By a reduction in the length of the prism the crystals become more nearly equidimensional and sometimes assume a rhombic aspect. A still further reduction in the length of the prism gives a habit with a pyramidal development (Fig. 5), particularly if only *c* and *f* are the terminal faces and the prism is reduced to a point where these three faces join. The final habit, brought about by the reduction of the prism is a thin wedge-shaped crystal (Fig. 4). The presence of large pyramidal faces gives a habit unrelated to the usual one. The base and orthodomes are reduced to small size, the crystal being usually terminated by large but curved faces of $s(\bar{1}12)$ (Fig. 3).

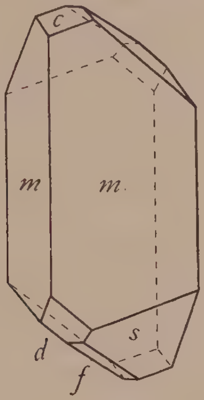

FIG. 3. Crystal of krausite with $c(001)$, $m(110)$, $d(\bar{1}01)$, $f(\bar{1}02)$ and $s(\bar{1}12)$.

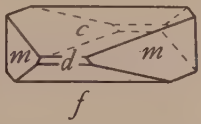

FIG. 4. Tabular crystal of krausite.

A gnomonic projection of the crystal forms is shown in fig. 6.

PHYSICAL AND OPTICAL PROPERTIES

The color of krausite is a pale yellowish green. The crystals are nearly pale turtle green (Ridgway) while the aggregated crystals are somewhat more gray, approaching lichens green. The luster is a bright vitreous one. Crystals are transparent and often flawless. Streak white. There are two good cleavages, the basal one being perfect and the mineral readily splits along this direction into thin plates. A second cleavage parallel to *a*(100) is good; the combination of these two cleavages causes the mineral to be easily broken into rods and shreds. The hardness is 2.5. The specific gravity, determined by floating clear crystals in a mixture of methylene iodide and carbon tetrachloride was found to be 2.840.

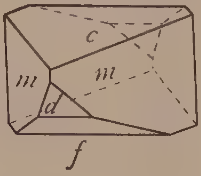

FIG. 5. Pseudo-pyramidal crystal of krausite.

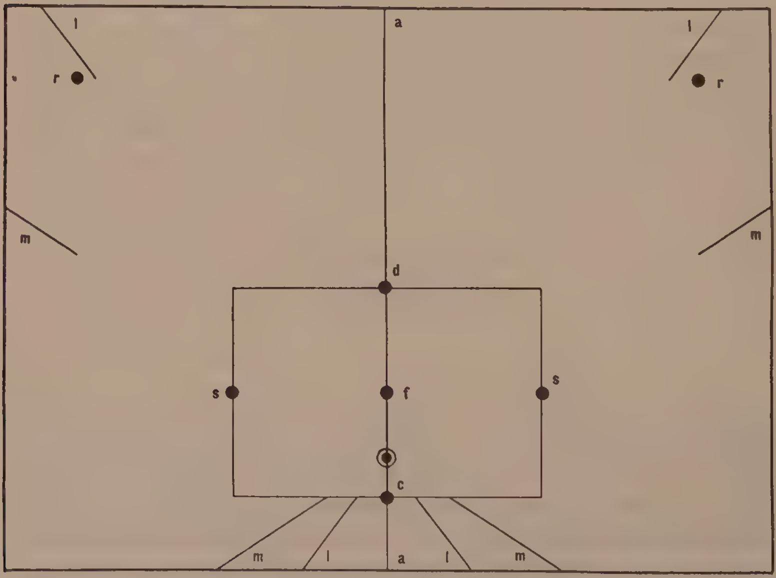

FIG. 6. Gnomonic projection of krausite forms.

Optically krausite is biaxial, positive, with a very large optic axial angle. The indices of refraction were found to be: $\alpha=1.588$, $\beta=1.650$, $\gamma=1.722$. The birefringence is high and the crushed fragments show numerous bands of color. The plane of the optic axes is normal to the plane of symmetry and the optical orientation is: $Z=b$, $X \wedge c=35^\circ$. The optical orientation is shown in fig. 7. The pleochroism is weak but distinct in the thicker grains: $X=$ colorless; Y and Z = pale yellow. Basal cleavage sections show no appreciable pleochroism and no distinct optical figure. The crystals lying on the prism show the emergence of an optic axis just at the edge of the field, while the crystals lying on the clinopinacoid edge show the maximum extinction and an optical figure with a wide separation of the optic axes.

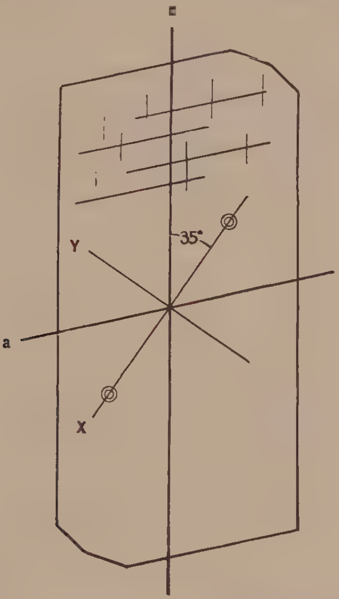

FIG. 7. Optical orientation and cleavage of krausite.

Due to paucity of material and unsatisfactory character of the mineral from Velardena, it was not studied in detail. Krausite from here is found as fine, drusy crusts of crystals of a pale greenish yellow color on blocks and in cracks in limestone, associated with voltaite, halotrichite and other iron minerals. The mineral has resulted from the oxidation of a considerable quantity of pyrite thrown on the dump many years ago. This pyrite has given rise to a series of iron sulfates, of which copiapite is the most common. The krausite is confined to the material in close association with the fragments and blocks of limestone. The crystals are too small for crystallographic determination but the general appearance of the mineral, the approximate determination of its optical properties, its insolubility in water and its other chemical characters identify it quite satisfactorily as krausite.

THE CRYSTAL STRUCTURE OF MARCASITE

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ABSTRACT

The only attempts to investigate the crystal structure of marcasite have been made by Huggins and by de Jong. Huggins' contribution has been of the nature of guesswork. The structure proposed by him on the basis of Lewis' atomic theory ultimately proves correct, although his crystallographic substantiation of it is fortuitous and incorrect. De Jong, who attempted the only x-ray work on marcasite, arrived at dimensions for the unit cell similar to those given beyond, except that his a-axis is doubled. He gave V_h^{11} as the space group.

In this paper, the details of a complete x-ray determination of the structure of marcasite are given. No essential assumptions have been made other than that marcasite is holohedral. The rotation and oscillation method of analysis was alone used, with the crystal completely bathed in molybdenum Kα radiation. The determination leads to the following structure for marcasite:

Unit cell: $a=3.37$ Å
$b=4.44$ Å
$c=5.39$ Å

Space group: V_h^{12}

Iron atoms (on symmetry centers) at: $[[000]]$ and $[[\frac{1}{2}\frac{1}{2}\frac{1}{2}]]$

Sulfur atoms (on reflection planes) at: $[[Ou_bv_c]]$, $[[O\bar{u}_b\bar{v}_c]]$,
$[[\frac{1}{2}, \frac{1}{2}-u_b, \frac{1}{2}+v_c]]$, and $[[\frac{1}{2}, \frac{1}{2}+u_b, \frac{1}{2}-v_c]]$

where $$\begin{cases} u_b = .203 \pm .01 \\ v_c = .375 \pm .01 \end{cases}$$

(Conventional marcasite orientation, origin at a symmetry center).

There is no complete agreement among the authors giving analytical expressions or equivalent positions of V_h^{12}. The equivalent positions are therefore rederived. It proves that Schiebold gives incorrect positions for symmetry centers and screw axes, and that Mark gives an incorrect origin of coordinates for the equivalent positions of this space group.

Marcasite possesses a 6–3 coordination structure. It is made up of units essentially equivalent to units discernable in the pyrite structure. Pyrite has a different linking of the groups which is also consistent with 6–3 coordination. The rutile structure is a special case of the marcasite structure, and the rutile and marcasite groups display a very similar crystal habit.

Marcasite appears to be composed of iron and sulfur in the atomic state. Both kinds of atoms have almost identical radii, 1.12 Å.

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LITERATURE

Since almost the beginning of the period of crystal analysis with aid of x-rays, the structure of pyrite has been known. Indeed it was the first crystal species analyzed,[1] all of whose atoms were not fixed by symmetry. The structure of its polymorph, marcasite, however, has continued to remain unknown, although it has been guessed at, and an attempt has made to deduce it by x-ray means.

Believing that the Lewis theory of the structure of the atoms required the linking of sulpher and iron atoms to be the same in pyrite and marcasite, Huggins[2] presented a structure for marcasite

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[1] W. Lawrence Bragg, The Analysis of Crystals by the X-ray Spectrometer: *Proc. Royal Soc. London*, (A) **89**, 1914, pp. 476–478.

[2] Maurice L. Huggins, The Crystal Structures of Marcasite (FeS_2), Arsenopyrite (FeAsS), and Loellingite ($FeAs_2$): *Physical Review*, (2) **19**, 1922, pp. 369–373.

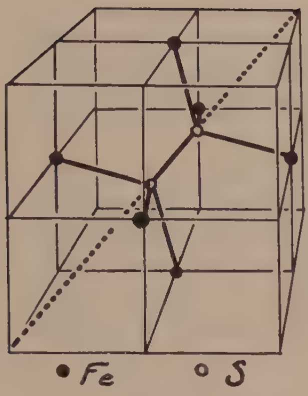

FIG. 1A. Huggins' Fig. 1A very slightly modified: the arrangement of iron atoms about the S–S group in pyrite.

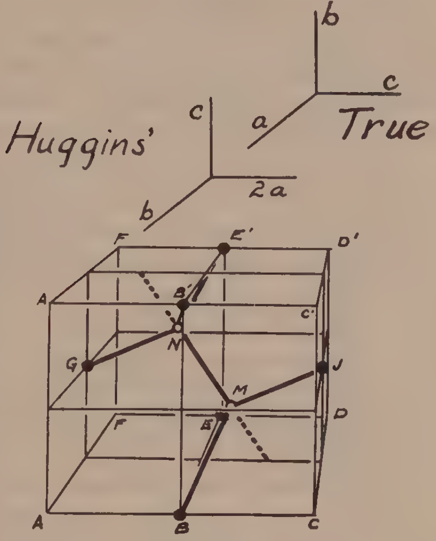

FIG. 1B. Huggins' Fig. 1B, very slightly modified: the arrangement of iron atoms about the S–S group in marcasite. The directions of the conventional marcasite axes are shown in comparison with those deduced by Higgins.

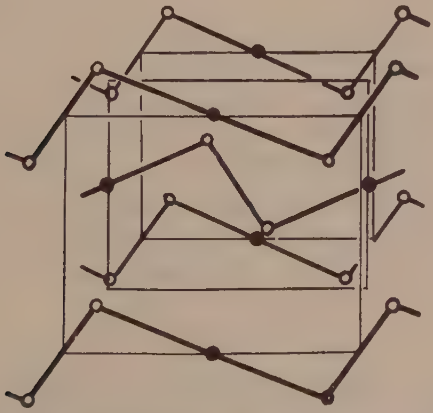

FIG. 2. Huggins' Fig. 2, somewhat modified, illustrating the orthorhombic structure resulting from continuing the arrangement implied in Fig. 1A.

based on a rearrangement of major units of the pyrite structure. Since the structure so deduced has actually proven to be correct, Huggins' figures are reproduced here. It should be pointed out that Huggins' crystallographic substantiation of this structure is totally incorrect.

Fig. 1A illustrates the arrangement about the S–S group in pyrite. By reorienting this group undisturbed, as in Fig. 1B, and linking the groups as in Fig. 2, an orthorhombic structure results. The rearrangement of groups leaves the requirements of Lewis' theory satisfied.

In attempting to justify this structure, Huggins' argument is that the axial ratio of marcasite given by Allen, Crenshaw, Johnston, and Larsen,[3] namely 0.7646:1:1.2176, is consistent with the ratio of lengths $AB:AF:AA'$, Fig. 1B. Hence, he decides, these are the directions of the a, b, and c crystallographic axes, respectively. Since the unit cell, Figs. 1B and 2, is double the length of AB in the direction of this line, the true axial ratio of marcasite, Huggins concludes, should be: 1.5292:1:1.2176.

The fact is, however, that Huggins does not have the correct orientation. The x-ray work to be described later proves the sulfur atoms to occupy (100) planes, hence, Huggins' b is equivalent to crystallographic a. Trial calculation indicates that the axes must transform as follows:

Huggins		Crystallographic
b	is actually	a
c	is actually	b
$2a$	is actually	c

Using the axial ratio data adopted by Huggins, his axial ratio $\overset{c}{1.5292}:\overset{a}{1}:\overset{b}{1.2176}$ should actually be $\overset{a}{1}:\overset{b}{1.2176}:\overset{c}{1.5292}$, or .822:1:1.256, which is fairly close to the marcasite ratio. In other words, Huggins' incorrect, apparent substantiation for the proposed structure depends on the fortuitous relation between the marcasite axes:

$$a:b:c \stackrel{\frown}{=} b:c:2a$$

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[3] E. T. Allen, J. L. Crenshaw, John Johnston, and Esper S. Larsen, Die mineralischen Eisensulfide: *Zeit. Anorg. Chemie*, **76**, 1912, p. 254. This is equivalent to the more familiar article in English by the authors: *Am. J. Sc.*, (4) **33**, 1912, p. 221.

The only experimental attempt to determine the structure of marcasite has been made by de Jong.[4] De Jong attempted to analyse a crystal of marcasite from "Bohemia," with Fe-K radiation using only the powder method.[5] He also partially investigated other minerals of the marcasite group by both powder and rotating crystal methods. His results may be summarized as follows:

Axial lengths of unit cell			Formula weights per unit cell	Density		Space group
				Calculated	Literature	
a 6.79Å	*b* 4.45Å	*c* 5.42Å	4	4.86	4.85–4.90	V_h^{11}

De Jong did not attempt to complete the structural determination.

MATERIAL

All of the writer's experimental work was done on crystals derived from a single hand specimen. Although unlabeled, this was one of the familiar Joplin specimens showing a thin chert sheet on both sides of which had grown deep wine-colored sphalerite crystals, which in turn, had acted as a focus for the crystallization of marcasite. This particular specimen was chosen because its marcasite crystals, on the whole, were homogeneous, easily oriented, and provided untwinned individuals.

The marcasite crystals themselves were of diamond shaped, tabular habit, flattened parallel to $\{001\}$. The diamond shape was outlined by $\{110\}$. The basal pinacoids were not actually present, but were represented by slightly warped, highly striated surfaces of this altitude, produced by vicinal brachydome striations. None of the planes of the striations were identified with certainty, but some of the $\{110\}$ planes gave fairly good signals. The average of several measurements on one crystal gave:

$$(110) \wedge (\bar{1}10) = 105° \ 42'$$

from which it follows: $a:b = .7577:1$

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[4] W. F. de Jong, Bepaling van de absolute aslengten van markasiet en daarmee isomorfe mineralen: *Physica*, **6**, 1926, pp. 325–332.

[5] *Op. cit.* p. 329 and p. 331.

A personal determination of the density on about .7 gram of carefully hand picked, crystal fragments of this material gave a value of 4.919 at 28° C.

Delicate qualitative[6] determinations[7] on a total of about .8 gram of this marcasite indicated that nickle and cobalt (elements to be expected as possible constituents replacing some iron) as well as antimony, arsenic, and bismuth (to be expected as possible replacers of some sulfur) are absent. Incidentally, lead and copper were also found to be absent. Allen, Crenshaw, Johnston, and Larsen[8] found the marcasite from Joplin to be of ideal FeS_2 proportions. Doelter and Leitmeyer[9] quote an analysis of Missouri marcasite by E. Arbeiter which also indicates ideal FeS_2. The marcasite used in the structural determination, therefore, may be regarded as perfectly suited for the establishment of a new crystal structure type.

The absorption coefficient of marcasite is high, consequently relatively minute splinters were used in the x-ray determinations. Three crystals were used, mounted for rotation about the a, b, and c axes, respectively. Because of the poor but real cleavage along $\{110\}$, the c axis splinter was most nearly of uniform cross section, and was used for most of the intensity comparisons.

THE UNIT CELL

All x-ray work was done by means of the rotation and oscillation methods, following Bernal[10] rather closely, with the crystals completely bathed in molybdenum Kα radiation. The axial lengths were determined by rotating the crystals about the three crystallographic axes and recording the reflection on $3\frac{1}{4}\times 4\text{-}\frac{1}{4}$ inch glass plates at a distance of about 6 cm. from the crystal. The following values were obtained:

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[6] I was prepared to have quantitative analyses made, but our best professional analysts (including Miss Mary G. Keyes and the new laboratory for rock analyses in charge of Dr. Grout of the University of Minnesota) declined to make them, pleading inadequate equipment for sulfide analyses. Where can one obtain reliable sulfide analyses? My own experience with the routine commercial analyst is that he cannot be relied upon for scientific work.

[7] G. G. Marvin, analyst.

[8] E. T. Allen, J. L. Crenshaw, John Johnston, and Esper S. Larsen, The Mineral Sulfides of Iron: *Am. J. Sc.*, (4) **33,** 1912, p. 177.

[9] C. Doelter and H. Leitmeyer, *Handbuch der Mineralchemie*, Bd. **IV,** Erste Hälfte, Dresden and Leipzig, 1926, p. 567, analysis 8.

[10] J. D. Bernal, On the Interpretation of X-Ray, Single Crystal, Rotation Photographs: *Proc. Royal Soc. Lond.*, (A) **113,** 1926, pp. 117–160.

$$a = 3.37\text{Å}$$
$$b = 4.44\text{Å}$$
$$c = 5.39\text{Å}$$

In view of the fact that de Jong had already published an *a*-axis length about double that just given, special attention was given to the possibilities of an error in this determination. Of course, it is easy to overlook half-spaced, odd value, layer lines, and usually any mistake made in obtaining axial lengths is in the direction of missing these and obtaining halved axes. It is quite certain, however, that none of these appeared in any of the writer's photographs. These photographs include not only ordinary rotation plates placed at a distance of about 6 cm., and exposed about 17 hours, but also longer exposures of 40 hours, both at about 6 cm. with flat plates, and at about 5 cm. with cylindrical film. None of the 17 hour exposure, 15° oscillation showed any indications of missed layer lines, and, finally, every reflection was indexed without difficulty, none requiring a halved *a*-axis reciprocal lattice (*i.e.*, a doubled *a* axis in the space lattice).

	Axial Ratio *a*:*b*:*c*		Density
x-ray determination	.759:1:1.214	calculated from *x*-ray data	4.91
goniometric determination	.758:1: ?	actually determined	4.92
Goldschmidt's average[11]	.758:1:1.212		
Larsen, synthetic[12]	.7646:1:1.2176		
		Dana's range	4.85–4.90

The number of formula weights of FeS_2 associated with a unit cell may be calculated as

$$z = \frac{\text{Volume} \times \text{density}}{\text{Formula weight} \times 1.64 \times 10^{-24}}$$
$$= \frac{(3.37 \times 4.44 \times 5.39) \times 10^{-24} \times 4.92}{119.96 \times 1.64 \times 10^{-24}} = 2.03,$$

indicating two formula weights per unit cell.

[11] From Victor Goldschmidt, Winkeltabellen, *Berlin*, 1897, pp. 232, for which Goldschmidt says (page 413), "The elements differ strongly according to various observers. The mean of the data by Miller, Sadebeck, and Gehmacher are given."

[12] E. T. Allen, J. L. Crenshaw, John Johnston and Esper S. Larsen, The Mineral Sulphides of Iron. *Am. J. Sc.*, (4) **33**, 1912, p. 221.

The values of this axial ratio and the density calculated from it are in good agreement with the goniometrically determined ratio and the direct density determination shown in table on page 367.

The differences between the axial ratios given and those found in the literature need not be dwelt upon. The axial ratio is unquestionably a function of the composition. The check between Goldschmidt's average and my own values is probably fortuitous.

Table I
Catalog of Planes Indexed

Pinacoids

h00	*0k0*	*00l*
—	—	—
200	—	**002**
—	—	—
400	**040**	—
—	—	—
600	060	006

Prisms and domes

hk0	**110**	—	**310**	—	510	—	710
	—	—	—	—	—	—	
	—	—	—	—	—		
	—	240	—	440	—	640	
	150	—	350	—	550		
	—	260	—	460			
	—						
	—						
	190						
h0l	**101**	—	—	—	—	—	701, or 711
	—	**202**	—	402	—	602, or 612	
	103	—	303	—	503	—	
	—	—	—	—	—	604, or 614	
	105	—	305	505, or 515			
0kl	**011**	**021**	**031**	**041**	—	061	071
	012	**022**	**032**	**042**	—	062	072
	013	**023**	**033**	**043**	053	063	084
	—	**024**	—	044	—	064	084
	015	025	—	045	055		

TABLE I (*Cont'd.*)
Catalog of Planes Indexed

Pyramids					*h5l*			
1kl	**111**	**121**	**131**	**141**	—	161	—	181
	112	**122**	**132**	**142**	152	162	172	
	113	**123**	**133**	143	—	163		
	114	—	**134**	—	—		164	
	115	—	135	145	—	165		
2kl	**211**	**221**	**231**	241	—	261	271	
	212	**222**	**232**	242	—	262	—	282
	213	**223**	**233**	243	253	263		
	—	**224**	—	244	—	264	—	284
	215	225	—	245	—	265		
3kl	**311**	**321**	331	341	—	361		381
	312	**322**	332	342	352	362		
	313	—	333	343	—	363		
	314	—	334	—	—	—	374	
	315	—	—	345	—	365		
4kl	411	421	431	441	—	—	471	
	412	422	—	442	—	462		
	413	—	—	443	453			
	—	424	—	444	—			
	415	—	—	445	455			
5kl	511	521						
	512	522	532	542	552			
	513	—	—	543				
			534					
	515, or							
	505							
6kl	—	—	631					
	612, or	622?						
	602							
	613							
	614, or	624						
	604							
7kl	711, or	721, or						
	701	711						

THE SPACE GROUP

INDEXING. Following Bernal,[13] the planes giving rise to reflections have been indexed by allowing the crystal to oscillate through definite 15° ranges, with an overlap of 2° between range settings. Sets of photographs were thus made for oscillations about the *a*, *b*, and *c* axes, recording being accomplished on flat plates at about 6 cm. crystal-to-plate distance. The planes so indexed are listed in heavy type in Table I. The chance of mis-indexing among these planes is very slight, for most of them appeared on all three axial sets of oscillations, and were therefore checked twice, while all but a very few appeared on at least two axial sets of oscillations.

In order to fix the sulfur parameters more closely, it was necessary to obtain reflections from planes of higher index than those recorded on the $3\frac{1}{4}\times4\frac{1}{4}$ plates at about a 6 cm. plate distance. For this purpose, a complete new set of oscillation and rotation photographs was made using a cylindrical camera of about a 5 cm. radius. All plates so indexed are listed in Table I in ordinary type. It is believed that the indexing is correct except for possibly some of the very high index planes where the oscillation range allowed a choice between two possibilities. In most cases, the doubt and choice have been indicated in the table.

The plane 006 alone was indexed from a complete rotation photograph by correlation of reflection sequence.

DETERMINATION OF SPACE GROUP. An analysis of the recorded reflections indicates that all classes of pyramid planes (*hkl*) are present regardless of the values of $h+k$, $h+l$, $k+l$, or $h+k+l$. Hence the space lattice can not be (001)-centered, (010)-centered, (100)-centered, face-centered, or body-centered. It must therefore be the simple orthorhombic lattice Γ_0. This eliminates all orthorhombic space groups except:

$$C_{2v}{}^1 - C_{2v}{}^{10},\ V^1 - V^4,\ V_h{}^1 - V_h{}^{16},$$

by reflections actually appearing.

Of the pinacoids, prisms, and domes, the reflection of the following classes of planes only are absent:

(a) (*hk*0) when $h+k$ is odd
(b) (*h*0*l*) when $h+l$ is odd

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[13] *Op. cit.*

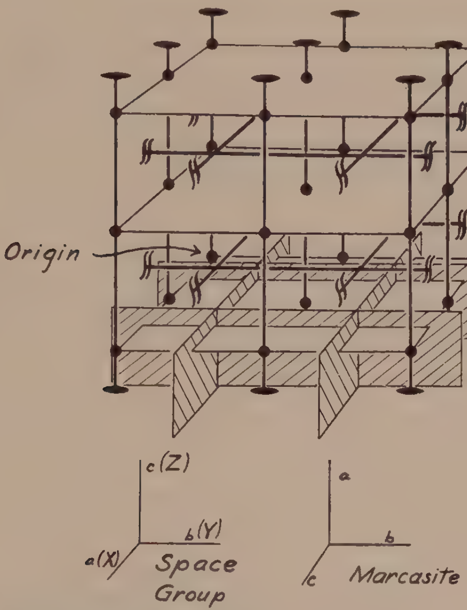

FIG. 3. Perspective view of space group V_h^{12}, with both conventional space group orientation and conventional marcasite orientation indicated. The symmetry elements are as follows: horizontal reflection planes; vertical glide planes with diagonal glides; vertical 2-fold rotation axes; horizontal 2-fold screw axes; and symmetry centers.

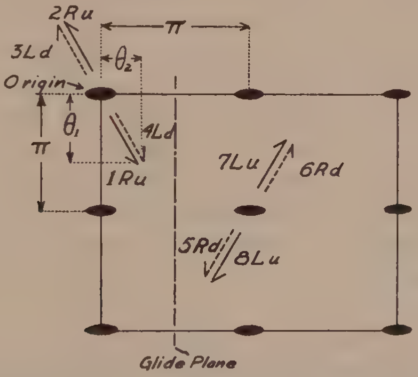

FIG. 4. Projection of some of the symmetry elements of V_h^{12} on the lower reflection plane of Fig. 3, illustrating the derivation of the coordinates of the general position by the use of the reflection planes, the $(010)_{\text{space group}}$ diagonal glide planes, and 2-fold axes.

(c) (*h00*) when h is odd
(d) (*0k0*) when k is odd
(e) (*00l*) when l is odd
special cases of (a) and (b)

Reflection of all other classes of planes are present. This eliminates all of the above space groups except:

$$C_{2v}^{1},\ C_{2v}^{7},\ C_{2v}^{10},\ V^{1}, V^{2}, V^{3}, V^{4},\ V_{h}^{12},\ V_{h}^{13},$$

by reflections actually appearing.

In the rather complete list of reflecting planes available, no classes of planes (a) and (b) appeared, in spite of the fact that the dimensions and setup of the apparatus would have recorded, if present and if sufficiently intense:

at least 23 of the class (*hk0*) where $h+k$ is odd, including the special cases.

at least 17 of the class (*h0l*) where $h+l$ is odd, including the special cases.

It may reasonably be concluded, therefore, that these planes are absent because the classes are absent, and not because of some fortuitous condition. This eliminates all space groups but C_{2v}^{10} and V_h^{12}, both of which have absent classes identical with those observed. C_{2v}^{10} is hemimorphic, so, granting marcasite is holohedral, its space group is V_h^{12}.

In order to transform from the conventional space group orientation to the conventional marcasite orientation, the a and c axes are interchanged, together with the corresponding h and l indices.

EQUIVALENT POSITIONS OF V_h^{12}. A perspective view of space group V_h^{12} is given in Fig. 3. In Fig. 4, some of the elements of the group are shown projected on the lower, horizontal reflection plane of the perspective view of the space group. By introducing an assymmetric exploring "molecule" in a general position, the multiplication of this general "molecule" by the symmetry elements of the group can be studied for the purpose of deriving the equivalent positions of the group.

For coordinates, it is convenient, for x-ray intensity work, to use phase angles, in terms of which the length of any axis of the unit cell is 360° or 2π, half the length 180° or π, or, in general, any portion of the length is θ_n. The origin of coordinates used here is a symmetry center. By placing the "molecule" $1Ru$ in a general position, these elements reproduce it as indicated in Table II. Other elements than the particular ones chosen as generators in the tables could be used for deriving these equivalent positions. The symbols used in the projection can be comprehended from the following illustration: *6Rd* signifies "the 6th 'molecule', which is **R**ight handed, and pointing **d**own". It is convenient to conceive of "molecules" 1, 2, 3, and 4 as being clustered about the origin [[000]] and associated with the lower horizontal reflection plane, and of "molecules" 5, 6, 7, and 8 as being clustered about $[[\pi\pi\pi]] \approx [[\frac{1}{2}\frac{1}{2}\frac{1}{2}]]$ and associated with the next plane above. The dotted "molecules" are below the plane with which they are associated, the others are

Table II.

Derivation of Coördinates of General Position of V_h^{12}

Symmetry operation	"Molecule" operated upon	Designation of resulting "molecule"	Coordinates of resulting "molecule"	
			Space group orientation	Marcasite orientation
	original "molecule" 1	1*Ru*	$[[\theta_1\theta_2\theta_3]]$	$[[\theta_a\theta_b\theta_c]]$
Vertical 2-fold rotation axis through [[000]]	1	2*Ru*	$[[\bar{\theta}_1\bar{\theta}_2\theta_3]]$	$[[\theta_a\bar{\theta}_b\bar{\theta}_c]]$
Lower, horizontal reflection plane	2	3*Ld*	$[[\bar{\theta}_1\bar{\theta}_2\bar{\theta}_3]]$	$[[\bar{\theta}_a\bar{\theta}_b\bar{\theta}_c]]$
"	1	4*Ld*	$[[\theta_1\theta_2\bar{\theta}_3]]$	$[[\bar{\theta}_a\theta_b\theta_c]]$
Vertical glide plane with diagonal glide	4	5*Rd*	$[[\pi+\theta_1,\ \pi-\theta_2,\ \pi-\theta_3]]$	$[[\pi-\theta_a,\ \pi-\theta_b,\ \pi+\theta_c]]$
"	3	6*Rd*	$[[\pi-\theta_1,\ \pi+\theta_2,\ \pi-\theta_3]]$	$[[\pi-\theta_a,\ \pi+\theta_b,\ \pi-\theta_c]]$
"	2	7*Lu*	$[[\pi-\theta_1,\ \pi+\theta_2,\ \pi+\theta_3]]$	$[[\pi+\theta_a,\ \pi+\theta_b,\ \pi-\theta_c]]$
"	1	8*Lu*	$[[\pi+\theta_1,\ \pi-\theta_2,\ \pi+\theta_3]]$	$[[\pi+\theta_a,\ \pi-\theta_b,\ \pi+\theta_c]]$

TABLE III. SPECIAL POSITIONS OF V_h^{12}

Special Position	Coalescing "molecules"	Coordinates of coalesced "molecules"			Number of equivalent positions in special position	Wyckoff's designation of special position
		Space group orientation	Marcasite orientation	Wyckoff's coordinates		
"Molecules" on reflection planes	1+4 2+3 5+8 6+7	$[[\theta_1\theta_2 0]]$ $[[\bar{\theta}_1\bar{\theta}_2 0]]$ $[[\pi+\theta_1, \pi-\theta_2, \pi]]$ $[[\pi-\theta_1, \pi+\theta_2, \pi]]$	$[[0\theta_b\theta_c]]$ $[[0\bar{\theta}_b\bar{\theta}_c]]$ $[[\pi, \pi-\theta_b, \pi+\theta_c]]$ $[[\pi, \pi+\theta_b, \pi-\theta_c]]$	$[[uv\frac{1}{4}]]$ $[[\bar{u}\bar{v}\frac{1}{4}]]$ $[[u+\frac{1}{2}, \frac{1}{2}-v\ \ \frac{3}{4}]]$ $[[\frac{1}{2}-u, v+\frac{1}{2}, \frac{3}{4}]]$	4	*g*
"Molecules" on 2-fold rotation axes through [[000]]	1+2 3+4 5+6 6+7	$[[00\theta_3]]$ $[[00\bar{\theta}_3]]$ $[[\pi, \pi, \pi-\theta_3]]$ $[[\pi, \pi, \pi+\theta_3]]$	$[[\theta_a 00]]$ $[[\bar{\theta}_a 00]]$ $[[\pi-6_a, \pi, \pi]]$ $[[\pi+\theta_a, \pi, \pi]]$	$[[0, 0, \frac{1}{2}-u]$ $[[00u]]$ $[[\frac{1}{2}, \frac{1}{2}, u+\frac{1}{2}]]$ $[[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}-u]]$	4	*e*
"Molecules" on 2-fold rotation axes through [[0π0]]	1+2 3+4 5+6 7+8	$[[0\pi\theta_3]]$ $[[0\pi\bar{\theta}_3]]$ $[[\pi, 0, \pi-\theta_3]]$ $[[\pi, 0, \pi+\theta_3]]$	$[[\theta_a\pi 0]]$ $[[\bar{\theta}_a\pi 0]]$ $[[\pi-\theta_a, 0, \pi]]$ $[[\pi+\theta_a, 0, \pi]]$	$[[0, \frac{1}{2}, \frac{1}{2}-u]]$ $[[0\frac{1}{2}u]]$ $[[\frac{1}{2}, 0, u+\frac{1}{2}]]$ $[[\frac{1}{2}0\bar{u}]]$	4	*f*
"Molecules" on [[000]] symmetry center	1+2+3+4 5+6+7+8	$[[000]]$ $[[\pi\pi\pi]]$	$[[000]]$ $[[\pi\pi\pi]]$	$[[00\frac{1}{4}]]$ $[[\frac{1}{2}\frac{1}{2}\frac{3}{4}]]$	2	*a*
"Molecules on [[00π]] symmetry center	1+2+3+4 5+6+7+8	$[[00\pi]]$ $[[\pi\pi 0]]$	$[[\pi 00]]$ $[[0\pi\pi]]$	$[[00\frac{3}{4}]]$ $[[\frac{1}{2}\frac{1}{2}\frac{1}{4}]]$	2	*b*
"Molecules" on [[0π0]] symmetry center	1+2+3+4 5+6+7+8	$[[0\pi 0]]$ $[[\pi 0\pi]]$	$[[0\pi 0]]$ $[[\pi 0\pi]]$	$[[0\frac{1}{2}\frac{1}{4}]]$ $[[\frac{1}{2}0\frac{3}{4}]]$	2	*c*
"Molecules" on [[π00]] symmetry center	1+2+3+4 5+6+7+8	$[[\pi 00]]$ $[[0\pi\pi]]$	$[[00\pi]]$ $[[\pi\pi 0]]$	$[[\frac{1}{2}0\frac{1}{4}]]$ $[[0\frac{1}{2}\frac{3}{4}]]$	2	*d*

above the plane. By putting the exploring "molecule" *1Ru*, on the several symmetry elements of the space group instead of in a general, symmetryless position, it coalesces with one or more of its above seven derivatives, giving rise to the special positions listed in Table III.

A discussion of the space group and its equivalent positions has been given in some detail, for the following reasons:

1. In the most complete table of equivalent positions, that of Wyckoff,[14] there is no explicit means of knowing, so far as I can discover, what point has been used as the origin of coordinates. This may be obtained by a study of Wyckoff's figures, but only after the space group itself has been thoroughly visualized from some other source. When this has been done, the coordinates can be easily written down by inspection.

2. Mark, who published a list of equivalent positions,[15] lists positions identical with Wyckoff's, giving as the origin a symmetry center. This is incorrect. Both Wyckoff's and Mark's origins are evidently on 2-fold rotation axes halfway between symmetry centers. Hopeless confusion results if Mark's stated origin is relied upon for the deductions given beyond.

3. Schiebold[16] gives his origin of V_h^{12} as "on a twofold axis $\|$ [001] in intersection with a reflection plane $\|$ (001)," *i.e.*, on a symmetry center. He gives correct analytical positions of the reflection planes, glide planes, and 2-fold axes, but then fails to give any symmetry center at the origin or in equivalent positions. In fact, Schiebold's symmetry centers and screw axes are incorrectly located. Needless to say, this representation of the group is very misleading.

The best description of the space group and its equivalent positions is to be found in Niggli's work.[17]

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[14] Ralph W. G. Wyckoff, The Analytical Expression of the Results of the Theory of Space Groups: *Carnegie Institution of Washington, Publication No.* **318,** second edition, 1930.

[15] Hermann Mark, *Handbuch der angewandten physikalischen Chemie;* Bd. **14,** Die Verwendung der Röntgenstrahlen in Chemie u. Technik: Leipzig, 1926, pp. 460–461.

[16] Ernst Schiebold, Über eine neue Herleitung und Nomenklatur der 230 kristallographischen Raumgruppen: *Abhandlungen der mathematisch-physischen Klasse der Sächsischen Akademie der Wissenschaften,* Vol. **40,** No. 5, 1929, p. 88.

[17] Paul Niggli, Geometrische Kristallographie des Discontinuums, *Leipzig,* **1919,** pp. 198–199.

Possible Arrangements for Marcasite. Since there are two formula weights of FeS_2 per unit cell, two iron atoms and four sulfur atoms must be associated with each cell. Space group V_h^{12} has only 2-fold, 4-fold, and 8-fold positions available, therefore the iron and sulfur must be distributed as follows:

Irons in one of the four 2-fold positions, *a*, *b*, *c*, or *d*

Sulfurs either:
- by twos in the remaining 2-fold positions, *a*, *b*, *c*, or *d*,
- or by fours, in one of the three 4-fold positions, *e*, *f*, or *g*.

The total possible marcasite arrangements are therefore those shown in Table IV. Not all of these structures are different however. By changing the origin of coordinates of each of the sets of coordinate positions by π in the three axial directions, it becomes evident that a number of these combinations are identical, leaving only the following independent:

Symmetry determined		One parameter		Two parameter	
1	*abc*	13	*ae*	21	*ag*
2	*abd*	14	*af*	22	*bg*
3	*acd*	15	*be*	23	*cg*
		16	*bf*	24	*dg*

Finally, by allowing the variables θ_a, θ_b, and θ_c to assume all values between 0 and 2π, it can be shown that all possible marcasite structural possibilities can be represented by:

Symmetry determined		One parameter		Two parameter	
1	*abc*	13	*ae*	21	*ag*
2	*abd*	14	*af*		
3	*acd*				

This makes a total of no more than six possible structures.

TABLE IV. MAXIMUM NUMBER OF POSSIBLE MARCASITE STRUCTURES INDICATED BY SPACE GROUP

Combination number	Iron positions	Sulfur positions	
1	*a*	*bc*	12 symmetry-fixed structures. Sulfurs on symmetry centers
2	*a*	*bd*	
3	*a*	*cd*	
4	*b*	*ac*	
5	*b*	*ad*	
6	*b*	*cd*	
7	*c*	*ab*	
8	*c*	*ad*	
9	*c*	*bd*	
10	*d*	*ab*	
11	*d*	*ac*	
12	*d*	*bc*	
13	*a*	*e*	8 one-parameter structures. Sulfures on 2-fold rotation axes
14	*a*	*f*	
15	*b*	*e*	
16	*b*	*f*	
17	*c*	*e*	
18	*c*	*f*	
19	*d*	*e*	
20	*d*	*f*	
21	*a*	*g*	4 two-parameter structures. Sulfurs on reflection planes
22	*b*	*g*	
23	*c*	*g*	
24	*d*	*g*	

24 possible structures

INTENSITY CONSIDERATIONS

PHASE FUNCTION OF V_h^{12}. The amplitude of a wave scattered by a set of atoms in a unit cell, as a function of the positions of the atoms, may be represented by

$$P=\sum\nolimits_n e^{2\pi i}(h'\theta_1+k'\theta_2+l'\theta_3)$$

where, $\sum_n$ indicates a summation over the n atoms considered in the cell
e is the base of natural logarithms
$i=\sqrt{-1}$

$\theta_1, \theta_2, \theta_3$ are the phase coordinates of an atom
h', k', and l' are the index numbers of the plane reflecting.

If the crystal considered has a center of symmetry, the phase function may be more conveniently put into the following form by summing over half the total number of atoms, taking the coordinates in centrosymmetrical pairs:

$$P=\sum_{n/2} 2 \cos (h'\theta_1 + k'\theta_2 + l'\theta_3).$$

The particular form of the phase function for $V_h{}^{12}$ is then obtained by substituting the coordinates of general positions 1, 2, 6, and 7 (each one with its centrosymmetrical derivative understood) in this relation, which gives:

$$\begin{aligned}P=2\{&\cos (h'\theta_1+k'\theta_2+l'\theta_3)+\cos (-h'\theta_1-k'\theta_2+l'\theta_3)\\ &+\cos (h'[\pi-\theta_1]+k'[\pi+\theta_2]+l'[\pi-\theta_3])\\ &+\cos (h'[\pi-\theta_1]+k'[\pi+\theta_2]+l'[\pi+\theta_3])\},\end{aligned}$$

using space group orientation. This may be reduced to:

$$P=\begin{Bmatrix}8\\4\\2\end{Bmatrix} \cos (h\theta_a) \cdot\cos (k\theta_b) \cdot\cos (l\theta_c), \text{ where } h+k+l \text{ is even,}$$

and

$$P=-\begin{Bmatrix}8\\4\\2\end{Bmatrix} \cos (h\theta_a) \cdot\sin (k\theta_b) \cdot\sin (l\theta_c), \text{ where } h+k+l \text{ is odd,}$$

transformed to marcasite coordinates. $\begin{Bmatrix}8\\4\\2\end{Bmatrix}$ indicates that coefficient 8, 4, or 2 should be used corresponding to the number of atoms in the equivalent position considered.

REFLECTION INTENSITIES. The actual amplitude contribution of a set of atoms to the reflection of a plane is given by

$$s=F\cdot P$$

where P is the amplitude given previously and F is the scattering ability of the atom as a function of the angle between the incident and reflected beam. The F values used for the calculations involved in determining the structure of marcasite are given in Fig. 5. The curve for iron has been drawn directly from the data of Bragg and West.[18] The sulfur curve has been calculated by the method indicated by these authors.[19] The sulfur curve probably does not fall off as rapidly as it should, but for the relatively small values of sin θ employed in most of the calculations, it has given very satisfactory service.

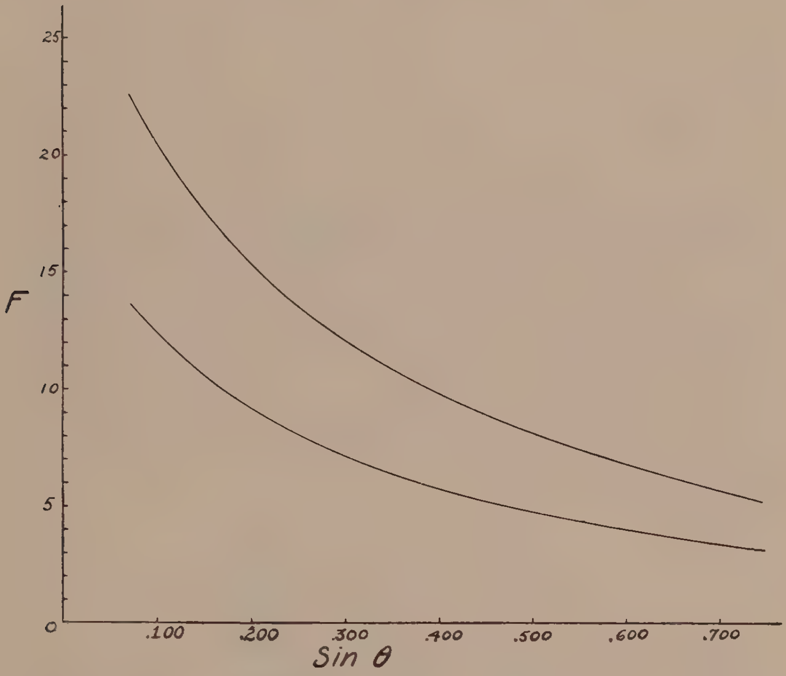

FIG. 5. The F values of iron (upper curve) and sulfur (lower curve) used in the determination of the structure of marcasite.

The amplitude contribution of all the atom species to the plane, or the structure factor, is

$$S=\sum s=\sum FP=F_{\text{iron}}\cdot P_{\text{iron}}+2F_{\text{sulfur}}\cdot P_{\text{sulfur}}$$

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[18] W. Lawrence Bragg and J. West, A Technique for the X-ray Examination of Crystal Structures with many Parameters: *Zeit. für Krist.*, **69**, 1928–1929, p. 139.

[19] *Op. cit.*, p. 137.

summed over all the atom species, in this case over iron and sulfur. The intensity of the reflection of a plane is given by[20]

$$I=\frac{1}{K^2}\cdot\frac{1+\cos^2 2\theta}{\sin 2\theta}\cdot S^2=\frac{1}{K^2}\cdot\Theta\cdot S^2$$

where K is a constant for a given apparatus and crystal specimen.

ELIMINATION OF IMPOSSIBLE MARCASITE STRUCTURES

INTENSITY COMPARISONS. The iron atoms of marcasite occupy symmetry-fixed positions, and the sulfur atoms occupy positions of no more than two undetermined parameters. It is possible, therefore, to calculate the intensities of reflections of various orders to be expected from one pinacoid for the two parameter structures, for two pinacoids for the one parameter structures, and for all three pinacoids from the symmetry-fixed structures. Comparison with the intensities actually observed then allows structures to be eliminated which do not give sequences of intensities indentical with those observed. The observed orders of intensities for the pinacoids are as follows:

200	>	400	>	600
strong		medium		weak
040	>	060	>	020
medium		weak		absent
002	>	006	>	004
strong		medium		absent

In Table II, the intensities (in the convenient form $|K\sqrt{I}|$), calculated for the different possible arrangements, are compared with those observed. Only the two parameter structures,

$$21\text{–}24: \left|\begin{matrix}a\\b\\c\\d\end{matrix}\right|_{\text{iron}}\cdot g_{\text{sulfur}},$$

give intensity orders not in conflict with those actually observed. Since all these structures are identical, they may be represented by the single structure $a_{\text{iron}}\ g_{\text{sulfur}}$.

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[20] W. Lawrence Bragg and J. West, *op. cit.*, p. 125.

THE MARCASITE STRUCTURE. From the above considerations it is evident that the iron atoms occupy symmetry centers while the sulfurs lie in reflection planes. The structure can be represented by the following coordinates:

Irons at $[[000]]$ and $[[\pi\pi\pi]]$
Sulfurs at $[[0\theta_b\theta_c]]$, $[[0\theta_b\theta_c]]$, $[[\pi,\pi-\theta_b,\pi+\theta_c]]$, $[[\pi,\pi+\theta_b,\pi-\theta_c]]$.

It remains now to determine the values of the parameters θ_b and θ_c.

DETERMINATION OF PARAMETERS

The two parameters, θ_b and θ_c have been fixed by independently finding a value of each, for which all planes not involving the other variable give calculated intensities in the same order as the observed intensities. All intensity comparisons, except as specifically

TABLE V. OBSERVED PINACOID INTENSITY ORDERS COMPARED WITH CORRESPONDING INTENSITIES CALCULATED FOR POSSIBLE MARCASITE STRUCTURES

Plane	Calculated Intensities $\lvert K\sqrt{I}\rvert$			Observed Intensities
	Arrangements 1–12	Arrangements 13–20	Arrangements 21–24	
200	139	Variable with θ_a	139	Strong
400	56		56	Medium
600	28		28	Weak
020	186	186	Variable with θ_b	Absent
040	83	83		Medium
060	45	45		Weak
002	225	225	Variable with θ_c	Strong
004	107	107		Absent
006	61	61		Medium

noted beyond, were made on a single *c* axis, complete rotation photograph using a cylindrical camera (Fig. 6). This allows all intensities to be compared with one another.

In a preliminary way, it is evident from the intensity order:

110	>	040	>	060	>	020,
very strong		medium		weak		absent

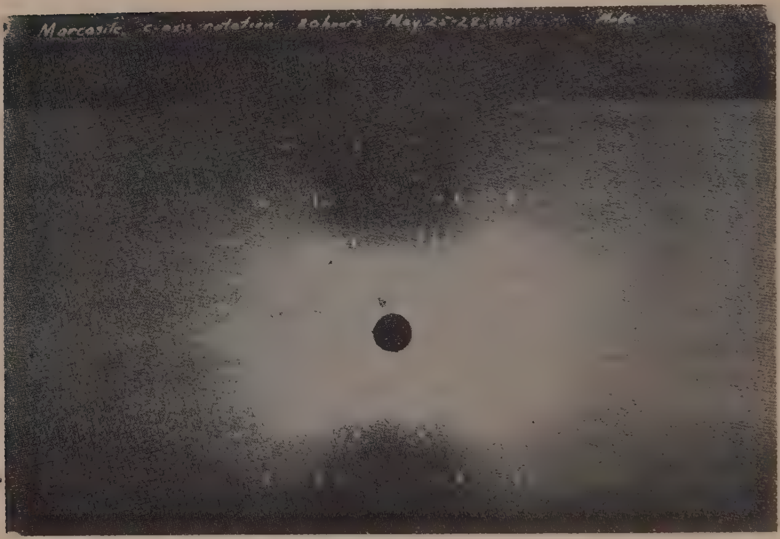

FIG. 6. Print of marcasite *c* axis rotation photograph. The fogging is due to *x*-rays scattered backward by the paper covering of the film during a very long exposure.

that θ_b must lie in the general region near 70°, or in its centrosymmetrical region near 290°. The centrosymmetrical region may be temporarily neglected, since it simply indicates the position of the centrosymmetrical atom.

The variable θ_b is more closely fixed as indicated in Fig. 7, where the intensities of all planes not involving the other parameter, θ_c, are plotted as functions of the variable θ_b. At the bottom of the figure, some of the intensity relations which tend to limit the value of the parameter are indicated. θ_b is thus fixed at about 73° or 74° corresponding to $u_b = .203$ or $.205$, to within less than a percent of the total possible variation. It is interesting to note that this value is almost $u_b = \frac{1}{5}$ within the limits of accuracy of fixing θ_b.

As an indication of the correctness of the value of θ_b, the intensities calculated (graphically) at $\theta_b = 73°$ are listed in Table VI in comparison with the order of intensities observed on the *c* axis rotation photograph. The check is very satisfactory.

An additional check is had by studying the list of planes indexed (Table I). By examining the columns corresponding to the pyramids $(h5l)$, a type permitted by the space group for all values of h,k,l, $h+k$, $h+l$, $k+l$, and $h+k+l$, it is evident that only such planes reflect as have $h+k+l$ even. Out of at least ten chances for

TABLE VI. COMPARISON OF CALCULATED AND OBSERVED ORDERS OF INTENSITIES FOR $(hk0)$ PLANES, AT $\theta_b = 73°$

$\lvert K\sqrt{I}\rvert$	Plane	Observed order	
272	110	110	Very Strong
		V	
139	200	200	Strong
		V	
115	150	150	Strong
		V	
99	310	310, 240, 350, 040, 400	Medium
85	240		
80	350		
57	040		
56	400		
		V	
52	550	550	Moderately Weak
		V	
34	190	190, 640, 460, 710, 600, 060	Weak
32	640		
31	460		
29	710		
28	600		
26	060		
		V	
10	130	130, 330, 020, 530, 220, 420, 620, 170	Absent
6	330		
4	020		
3	530		
2	220		
2	420		
0	620		
0	170		

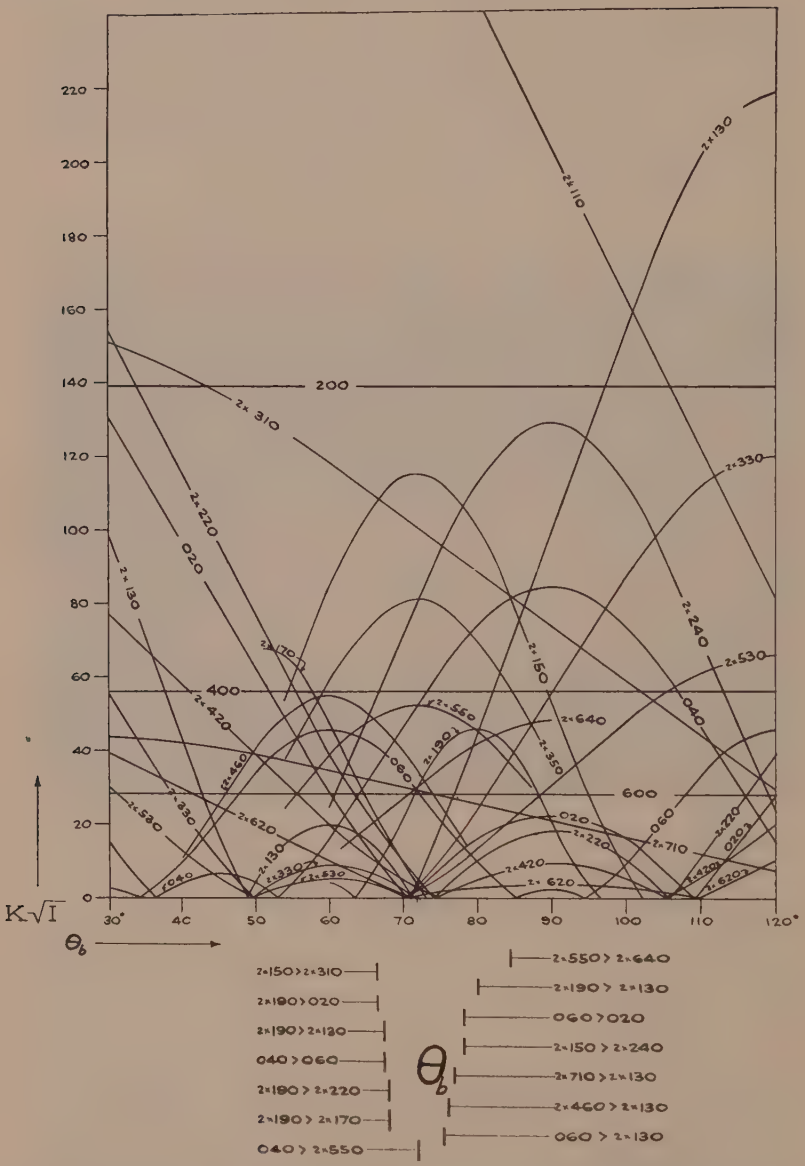

FIG. 7. The variations of intensity for all resolved planes within the dimensions of the apparatus for the c axis rotation and not involving θ_c, plotted as functions of the parameter θ_b. The notation $2\times hk0$ indicates that there are *two* pairs of planes in the form reflecting to the same spot on the photograph.

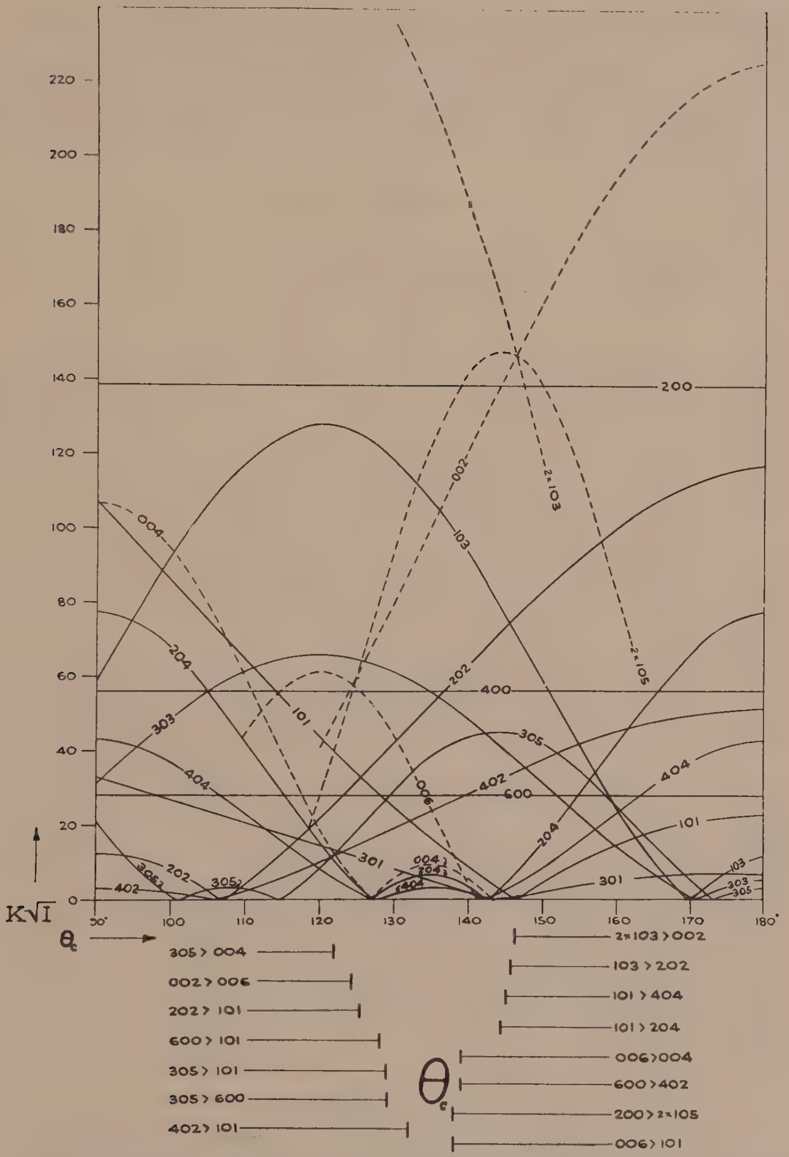

FIG. 8. The variations of intensity for all resolved planes within the dimensions of the apparatus for the c axis rotation, and not involving θ_b, plotted as functions of the parameter θ_c. The broken curves are additional intensity variations plotted for comparisons of the reflections of certain planes not appearing on the c axis rotation, but present on the a axis rotation. The notation $2\times h0l$ indicates there are *two* pairs of planes in the form reflecting to the same spot on the photograph.

planes with $h+k+l$ odd to reflect, not one reflection is recorded. There is no contribution by iron atoms to the reflections for which $h+k+l$ is odd, all diffracted radiation being due to the sulfur atoms. For marcasite, the phase function, P, for the sulfur atoms, takes the form:

$$P=-4\sin(k\theta_b)\cdot\sin(l\theta_c).$$

For planes ($h5l$), this is more specifically:

$$P=-4\sin(5\theta_b)\cdot\sin(l\theta_c).$$

Evidently the right hand member vanishes for any value of sin ($5\theta_b$) which is zero. This occurs when $5\theta_b$ is 0°, 180°, 360°, etc., or when θ_b is 0°, 36°, 72°, 108°, etc. The 72° solution corresponds with the θ_b determined graphically. Any value of θ_b very near to 72° would give rise to a sulfur contribution corresponding to an intensity too small to be detected on the photograph.

The parameter, θ_c, has been determined graphically (Fig. 8) in a manner similar to that used in the determination of θ_b. In addition, Fig. 8 shows the variation of certain planes (dotted curves) not appearing on the c axis rotation photograph, and whose observed intensity orders have been obtained from an a axis rotation photograph. The parameter θ_c is seen to be limited to 135°, corresponding to $u_c=.375=\frac{3}{8}$, to within less than one percent of the total possible variation. As an indication of the correctness of $\theta_c=135°$, the calculated intensities at this point in comparison with the observed order are given in Table VII. The correspondence is very good, taking into consideration the following point: reflections from planes located near the center of the rotation photograph, and on high layer lines always appear too intense, compared with calculated intensities. This is a normal condition, caused, in part, by the greater thickness of the splinter shaped crystal traversed by these beams. In no case has this effect seriously impaired the closeness of parameter determination.

An additional check on the correctness of θ_c is had by an inspection of the list of planes indexed (Table I). In the rows corresponding to ($0k4$) and ($hk4$), it is evident that only such planes reflect as have $h+k+l$ even. Out of at least fourteen chances for planes with $h+k+l$ odd to reflect, not one reflection is recorded. For this type

TABLE VII. COMPARISON OF CALCULATED AND OBSERVED ORDERS OF INTENSITIES FOR ($h0l$) PLANES, AT $\theta_c=135°$

$\|K\sqrt{I}\|$	Plane	Observed order	
		103	Very Strong
		V	
139	200	200	Strong
107	*103*	V	
56	400		
56	303	400, 303, 202, *305*	Medium
52	202	V	
38	*305*		
28	600	600, 402	Weak
24	402	V	
16	101	101	Very Weak
7	204	V	
5	301	204, 301, 404	Absent
3	404		

of plane, the total diffracted radiation is due to the sulfur atoms. In this case, the phase function takes the form

$$P=-4\sin(k\theta_b)\cdot\sin(4\theta_c).$$

The right hand member vanishes for values of $4\theta_c$ equal to 0°, 180°, 360°, etc., or for values of θ_c equal to 0°, 45°, 90°, 135°, 180°, etc. The 135° solution is identical with the value of the parameter already determined.

As final checks on the proposed parameters, Table VIII shows the graphically calculated and the observed intensities of planes not involving θ_c, and planes not involving θ_b, both taken together for comparison, and Table IX shows the calculated intensities of all planes having values of sin θ less than .4, and not near the central portion of the photograph. To include planes of higher values of sin θ would be to push the proof of accuracy of the parameters beyond the order of accuracy of their determination. The checks are clearly satisfactory.

THE MARCASITE STRUCTURE

DESCRIPTION. The considerations just detailed lead to a complete description of the structure of marcasite, in the following terms:

Unit cell: $a = 3.37$ Å
$b = 4.44$ Å
$c = 5.39$ Å

Space group: V_h^{12}

TABLE VIII. COMPARISON OF CALCULATED AND OBSERVED ORDERS OF INTENSITIES FOR (*hk0*) AND (*h0l*) PLANES, AT

$$\begin{cases} \theta_b = 73^\circ \\ \theta_e = 130^\circ \end{cases}$$

$\lvert K\sqrt{I}\rvert$	Plane	Observed order	
272	110	110, *103*	Very Strong
		V	
139	200	200	Strong
		V	
115	150	150	Strong
107	*103*		
99	310	V	
85	240		
80	350		
57	040	310, 240, 350, 040, 400, 303, 202, *305*	Medium
56	400		
56	303	V	
52	202		
52	550	550	
38	*305*		
34	190	V	
32	640		
31	460		
29	710	190, 640, 460, 710, 600, 060, 402	Weak
28	600		
26	060	V	
24	402		
16	101	101	Very Weak
10	130		
7	204		
6	330	V	
5	301		
4	020		
3	404	130, 204, 330, 301, 020, 404, 530,	
3	530	220, 420, 620, 170	Absent
2	220		
2	420		
0	620		
0	170		

Iron atoms (on symmetry centers) at: $[[000]]$ and $[[\frac{1}{2}\frac{1}{2}\frac{1}{2}]]$
Sulfur atoms (on reflection planes) at: $[[0u_bv_c]]$, $[[0\bar{u}_b\bar{v}_c]]$,

$[[\frac{1}{2},\frac{1}{2}-u_b,\frac{1}{2}+v_c]]$, and $[[\frac{1}{2},\frac{1}{2}+u_b,\frac{1}{2}-v_c]]$

$$\text{where} \begin{cases} U_b = .203 \pm .01 \\ V_c = .375 \pm .01 \end{cases}$$

$$\text{corresponding to} \begin{cases} u_b b = y_b = .900 \\ v_c c = z_c = 2.02 \end{cases}$$

TABLE IX. COMPARISON OF CALCULATED AND OBSERVED ORDERS OF INTENSITIES FOR ALL PLANES HAVING SIN θ UNDER .4 AND POSITIONS NOT TOO NEAR CENTER OF PHOTOGRAPH, AT

$$\begin{cases} \theta_b = 73° \\ \theta_c = 135° \end{cases}$$

$\|K\sqrt{I}\|$	Plane	Observed order	
272	110		
226	121	110, 121	Very Strong
151	231+041	V	
	unresolved	(231+041), 111, 200	Strong
147	111	unresolved	
139	200	V	
113	212		
109	321	212, 321, (132+222), *031*	Strong
102	132+222	unresolved	
	unresolved		
99	310	V	
89	131+221		
	unresolved		
86	*031*	310, (131+221), 240, 211, 040, 311	Medium
85	240	unresolved	
83	211		
60	311	V	
57	040		
37	021	021, 032	Weak
35	032		
16	101	101	Very Weak
10	130	V	
8	141		
5	301	130, 141, 301, 020, 220	Absent
4	020		
2	220		

for the marcasite studied. The coordinates are referred to the conventional marcasite orientation, taking the origin at a symmetry center.

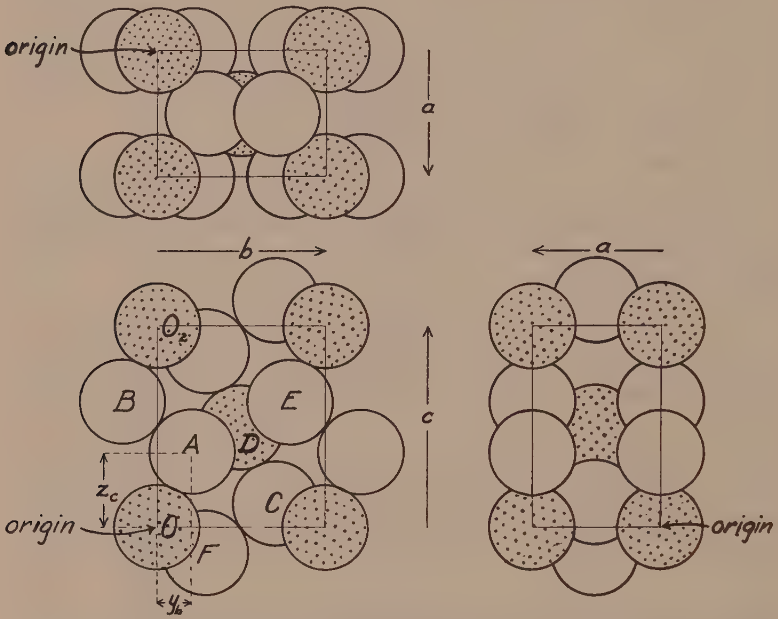

Fig. 9. (001)-plan (upper left), (100)-elevation (lower left), and (010)-elevation (lower right) of marcasite. The iron atoms (stippled) and sulfur atoms are drawn to scale. The relation between the sulfur pair and iron triad is well seen in the lower right (010) elevation. The bottom three irons form the triad, to which is attached, below and in back, the bottom two sulfurs. The axis of the sulfur pair slopes down and back away from the iron triad.

A unit cell of this structure, together with a few additional atoms to complete the picture, is shown in Fig. 9. The structure is identical with the one proposed by Huggins on grounds of atomic theory and shown in Fig. 2. From a certain point of view, it can be easily visualized as a stack of separate (100) planes; each plane consists of parallel strings of Fe–S–S–Fe–S–S– – – extending in the direction of the *c* axis with all the iron atoms in a straight line, but with the sulfur atom pairs nesting zigzag between these irons and causing the crooked appearance of the string. Adjacent threads have sulfur pairs pointing in the same direction, but adjacent planes have them pointing in reversed directions. Between (100) planes the fit is made by contacting an iron atom of one plane with the nearest sulfur atoms of neighboring strings in the next plane.

GEOMETRICAL PROPERTIES. Various important geometrical properties of the structure of marcasite can be calculated as follows:

Paired sulfur distance:

$$AB = \sqrt{(2y_b)^2 + (c - 2z_c)^2} = 2.25\text{Å}.$$

Unpaired sulfur distances:

$$AE = \sqrt{(b - 2y_b)^2 + (c - 2z_c)^2} = 2.96\text{Å}$$

$$AC = \sqrt{\left(\frac{a}{2}\right)^2 + \left(\frac{b}{2}\right)^2 + \left(2z_c - \frac{c}{2}\right)^2} = 3.10\text{Å}$$

$$AF = \sqrt{\left(\frac{a}{2}\right)^2 + \left(\frac{b}{2} - 2y_b\right)^2 + \left(\frac{c}{2}\right)^2} = 3.16\text{Å}$$

$$AA' \text{ (two (100) sheets apart)} = a = 3.37\text{Å}.$$

Iron—iron distances:

$$DD' \text{ (two (100) sheets apart)} = a = 3.37\text{Å}$$

$$OD = \sqrt{\left(\frac{a}{2}\right)^2 + \left(\frac{b}{2}\right)^2 + \left(\frac{c}{2}\right)^2} = 3.88\text{Å}$$

$$OO_2 = c = 5.39\text{Å}$$

$$DD_2' = \sqrt{a^2 + b^2} = 5.52\text{Å}$$

Iron—sulfur distances:

$$AO = \sqrt{y_b^2 + z_c^2} = 2.21\text{Å}$$

$$AD = \sqrt{\left(\frac{a}{2}\right)^2 + \left(\frac{b}{2} - y_b\right)^2 + \left(\frac{c}{2} - z_c\right)^2} = 2.24\text{Å}.$$

The structure displays 6–3 coordination. The iron atom, *D* is surrounded by six sulfurs at distances which are identical, within the accuracy of measurement: two sulfurs in the same plane, *C* and *G*, centrosymmetrical with respect to the iron; two in the plane in front, *A* and *E;* and two in the plane behind, centrosymmetrical with *A* and *E*. All these surround the iron at a distance of 2.21—2.24 Å. The sulfur atom, *A*, in turn, has three irons nearest it at this distance: *O*, in the same plane, and *D* and *D′* in the plane in front and behind.

The relation of the structure to other structures can best be visuallized by separating a sulfur pair with its immediate iron environment. This group, as indicated in Fig. 1B, is a sulfur pair capped at each end by an iron triad. The triangles formed by the iron triads are rotated 180° with respect to one another. These triangles are not exactly equilateral, but are rather isosceles, as indicated by the distances: $DD'=3.37$Å; OD and $OD'=3.88$Å; the acute angle is about $51\frac{1}{2}°$ instead of the ideal 60°. The angle which the plane of the iron triad makes with the direction of the sulfur pair is very close to the ideal 90°. For the parameters given, it can be calculated as:

$$180° - \tan^{-1}(b/c) - \tan^{-1}\left(\frac{y_b}{\frac{c}{2} - z_c}\right) = 87°.$$

RELATION TO OTHER STRUCTURES

PYRITE. These same units in the undistorted, ideally symmetrical condition are distinguishable in pyrite, and indeed it was on the assumption that these units carried over from pyrite to marcasite that Huggins[21] proposed a structure for marcasite. The difference between pyrite and marcasite is essentially one of a different linking of these units, at the same time satisfying the 6–3 coordination requirement.

In Table X certain geometrical properties of pyrite[22] are given in comparison with those of the marcasite structure, to bring out the essential identity of this common unit.

RUTILE. The rutile structure is a special case of the marcasite structure. The marcasite structure tends toward the rutile structure by decrease of the distance between the sulfur atom and the plane of the iron triad. When the sulfur atom actually occupies the plane of the iron triad, and the triad makes an angle of 90° with the sulfur pair, it is identical with the rutile structure type.

Proof of the close relation between the marcasite and rutile groups, as well as an excellent visual check on the general correctness of the marcasite structure, is offered in Fig. 10, in which standard crystal drawings of marcasite,[23] löllingite,[24] and rutile[25] are given in the same orientation for comparison. The tetragonaloid aspect of the marcasite group is obvious.

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[21] *Loc. cit.*

[22] Pyrite designations and distances taken from: P. P. Ewald and C. Hermann, *Structurber
icht*, 1913–1926, p. 153 (supplement to recent numbers of *Zeit. Krist.*).

TABLE X. COMPARISON OF CERTAIN DIMENSIONS OF THE COMMON UNIT OF THE PYRITE AND MARCASITE STRUCTURES

	Pyrite	Joplin marcasite
Paired sulfur distances	$d=2.10$Å	$AB=2.25$Å
Iron-iron distances in triad	$f=3.82$ $f=3.82$ $f=3.82$	$DD'=3.37$ $OD=3.88$ $OD'=3.88$
Distances from sulfur to irons in nearest triad	$e=2.26$ $e=2.26$ $e=2.26$	$AO=2.21$ $AD=2.24$ $AD'=2.24$
Distance from apex of one iron triad to centro-symmetrical apex	$a=5.40$ $a=5.40$ $a=5.40$	$c=5.39$ $DD_2=5.52$ $DD_2=5.52$
Angle between sulfur pair and iron triad	90°	±87°

THE CHEMICAL NATURE OF MARCASITE

RADII OF SULFUR AND IRON ATOMS. The geometrical properties listed indicate that the closest iron-sulfur approach is identical with the closest sulfur-sulfur approach, to within the limits of error of the determination. Slight changes in the parameters do not destroy the essential nature of this feature. Assuming that both the iron and sulfur atoms behave like rather hard spheres, it follows that they have the same radius, namely; about 1.12Å.

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[23] Traced from: Victor Goldschmidt, *Atlas der Kristallformen*, Heidelberg, **1920**, vol. 6.

[24] L. H. Bauer and H. Berman, Löllingite from Franklin, New Jersey, *Am. Mineral.*, **12**, 1927, p. 40.

[25] Habit taken from *Dana's System*, (1914), p. 238, Fig. 4, but redrawn so that the rutile c axis direction corresponds with the marcasite and löllingite a axis direction, and the rutile a_1 and a_2 axial directions corresponding with the marcasite and löllingite b and c axial directions.

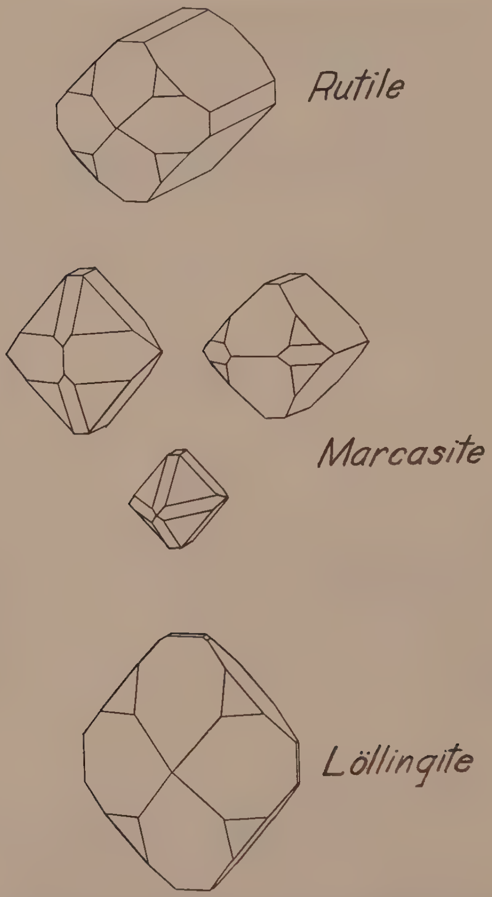

Fig. 10. Comparison of the habits of the rutile and marcasite groups. As redrawn, the rutile *c* axis is parallel with the marcasite and löllingite *a* axis direction. Other axes are parallel. Corresponding faces, referred to this orientation, have identical indices.

State of Ionization. The probable state of ionization of the atoms in marcasite may be investigated without any chemical assumptions whatever by considering the sulfur-iron spacing to be expected from sulfur atoms and iron atoms in various states of ionization. The situation may be appreciated at a glance, thus:[26]

[26] Radii from: V. M. Goldsmidt, Geochemische Verteilungsgesetze der Elemente, vol. 7: *Skrifter utgitt av Det Norske Videnskaps-Akademi i Oslo* I. *Matem.-Naturvid. Klasse*, **1926,** No. 2, pp. 26, 34, and 43.

	S^{6+}, .34Å	S^0, 1.04Å	S^{2-}, 1.74Å
Fe^0, 1.26Å	1.60Å	2.30Å	3.00Å
Fe^{2+}, 0.83Å	1.17Å	1.87Å	2.57Å
Fe^{3+}, 0.67Å	1.01Å	1.71Å	2.41Å

The figures are additions of the corresponding sulfur and iron radii. Evidently the only satisfactory chemical constitution for marcasite, from this geometrical criterion, is $Fe^0S_2^0$, which gives a sulfur-iron spacing of 2.30 Å, in rather good agreement with the observed spacing of 2.24 Å. The conclusion is that the sulfur and iron are in essentially the atomic state. The same situation also holds for pyrite, where this distance is 2.26 Å.

ACKNOWLEDGEMENT

It is a pleasure to acknowledge assistance from several sources. I am especially indebted to Prof. Palache of Harvard University for the gift of specimens of marcasite used in preliminary work, for placing at my diposal the use of the Harvard density determining apparatus, for permission to use the Harvard cylindrical camera for the rotating crystal method, and for many other courtesies rendered during the research. Mr. Berman of Harvard University also facilitated my work during the density determination.

I wish to thank my colleague, Prof. B. E. Warren, for permission to use the rotating crystal apparatus of the Department of Physics of the Massachusetts Institute of Technology, pending installation of suitable equipment in the Mineralogical Laboratories. Dr. Warren has also been kind enough to aid me at a number of points during my first working contact with the rotating crystal method.

This is the first of a series of papers dealing with the crystal structures of the marcasite group. The others, it is expected, will appear shortly.

CASTANITE, A BASIC FERRIC SULFATE FROM KNOXVILLE, CALIFORNIA*

AUSTIN F. ROGERS, *Stanford University*.

The status of castanite, a basic ferric sulfate with the formula $Fe_2O_3 \cdot 2SO_3 \cdot 8H_2O$, described from Sierra Gorda, Chile, by Darapsky[1] in 1890 is still in doubt. E. S. Dana[2] lists it as a distinct mineral, but Linck[3] states that castanite, along with paposite and hohmannite, is undoubtedly a synonym of amarantite ($Fe_2O_3 \cdot 2SO_3 \cdot 7H_2O$).

The study of some specimens recently collected at the old Redington or Boston quicksilver mine[4] at Knoxville, Napa County, California, furnishes data which indicate that castanite is a valid mineral species.

OCCURRENCE OF THE CASTANITE

My attention was called to the mineral here described, which was afterward identified as castanite, by Mr. George E. Gamble, owner and superintendent of the mine and one of my former students. Under Mr. Gamble's guidance I collected a number of castanite specimens from the footwall stope on the adit level in March 1930, and later Mr. Gamble kindly sent me additional material.

The castanite occurs in a brecciated impure opal replacement of serpentine which is known throughout the Quicksilver Region as "opaline."[5] In some of the specimens the castanite cements angular fragments of the opaline. A thin section of the opaline reveals opal as the principal constituent with some secondary chalcedony, disseminated pyrite and marcasite (metallic acicular crystals may be millerite), and relict grains of picotite from the peridotite stage.

Cinnabar and sulfur are directly associated with the castanite. All specimens contain minute well-formed sulfur crystals implanted on the castanite. A few of the specimens show cinnabar which occurs as a coating on the opaline fragments and seems to be earlier than the castanite.

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* Paper presented at the eleventh annual meeting of the Mineralogical Society of America, Toronto, Dec. 30, 1930.

[1] *N. Jb. f. Min.*, **1890**, 2, pp. 267–9.

[2] *System of Mineralogy*, 6th ed., p. 964, 1892.

[3] Hintze's *Handbuch der Mineralogie*, I Band, 32 Lief., pp. 4426–7, 1929.

[4] Also called the Knoxville mine.

[5] See *Bull.* **27**, *California State Min. Bureau*, p. 20, 1908.

The following sulfate minerals, copiapite, coquimbite, botryogen (palacheite), redingtonite, and knoxvillite, have been found at this mine. The writer has identified a fibrous ferric sulfate mineral from the footwall stope but not directly associated with the castanite as fibroferrite. This famous mine also furnished the type specimens of metacinnabar.

The castanite consists of a massive aggregate of minute subhedral crystals out of which there have grown clusters and single crystals of prismatic habit. The massive castanite has a beautiful "burnt-orange" color (Ridgway 11*j*, between orange rufous and Sanford's brown); the crystals are dark brown (Ridgway 10 *l*).

GEOMETRICAL CRYSTALLOGRAPHY

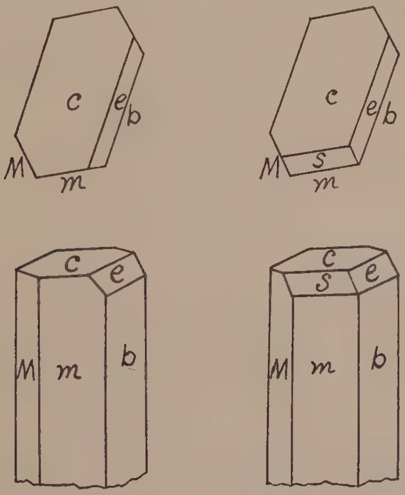

FIG. 1. FIG. 2.

FIGS. 1 and 2. Castanite crystals from Knoxville, California.

$b\{010\}$, $m\{110\}$,
$m\{1\bar{1}0\}$, $c\{001\}$,
$e\{011\}$, $s\{112\}$.

INTERFACIAL ANGLES OF CASTANITE

$(010)\wedge(110)=61°34'$ $(28', 33', 33', 38', 38')$
$(010)\wedge(110)=46\ \ 49$ $(42, 49, 50, 50, 56)$
$(001)\wedge(011)=42\ \ 32$ $(29, 31, 33, 34, 35)$
$(011)\wedge(010)=47\ \ 52$ $(46, 47, 54, 54, 60)$
$(001)\wedge(110)=89\ \ 10$ $(9, 10, 10, 11, 11)$

The crystals are prismatic in habit and on measurement prove to be triclinic. No doubly terminated crystals were found, but since positive and negative ends of different crystals have similar terminations the crystal class is probably pinakoidal. The crystals vary from about 2 mm. up to about 10 mm. in longest dimension. Six forms are present on the crystals examined. In order of prominence these are: $b\{010\}$, $M\{1\bar{1}0\}$, $m\{110\}$, $c\{001\}$, $e\{011\}$, and $s\{112\}$. Typical crystals are shown in Figs. 1 and 2. In habit the crystals are fairly constant. The only noteworthy variation is the relatively large size of the e faces on some crystals. The crystals are somewhat striated and etched and are not suitable for very accurate goniometric work. It was necessary to measure the three zones [001], [100], and $[1\bar{1}0]$ each on a different crystal. The measurements are given above (each the average of five). The (112) face was identified by the fact that it is common to the [001:110] and $[011:1\bar{1}0]$ zones. No good measurement could be obtained from this face.

From these five measured angles the following geometrical constants were calculated by spherical trigonometry:[6]

Geometrical constants of Castanite

$\alpha = 89°\ 50'$, $\beta = 91°10'$, $\gamma = 78°\ 46'$; $a:b:c = 0.726:1:0.895$. The calculations also yield the interfacial angles $(100) \wedge (010) = 101°14'$; $(001) \wedge (010) = 90°\ 24'$; $(100) \wedge (001) = 88°\ 48'$; and the interzonal angles $[001] \wedge [010] = 90°10'$; $[001] \wedge [100] = 88°50'$; $[001] \wedge [1\bar{1}0] = 90°54'$; $[001] \wedge [0\bar{1}1] = 48°16'$. The stereographic projection of castanite drawn on one of the convenient Penfield sheets is shown in Fig. 3. In order to obtain the geometrical constants it was necessary to solve the spherical triangles *cmb*, *amc*, and *abe*, first finding the angle *am* by the harmonic modification of the cotangent formula.[7]

In order to check the axial ratio a gnomonic projection (Fig. 4) was constructed from the measured and calculated angles. Penfield sheets may also be used for gnomonic projections since scale No. 2 of these sheets gives gnomonic degrees.

The faces are plotted and the prominent zone-lines are drawn. The center of the projection is z and a line zv normal to the zone-

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[6] I am indebted to my assistant, Dr. J. D. H. Donnay, for a careful checking of the computations.

[7] T. V. Barker, *Graphical and Tabular Methods in Crystallography*, p. 63, **1922.**

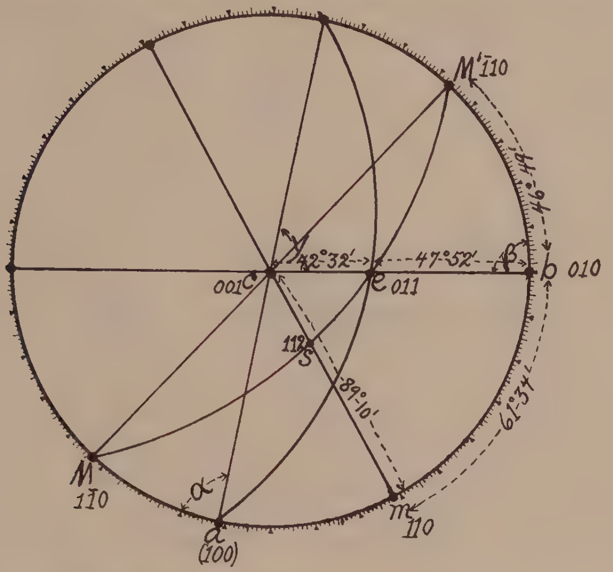

FIG. 3. Stereographic projection of castanite showing the five interfacial angles used in the calculations.

line [011:100] determines the point *v*. An arc with radius *zv* gives the point *x* on the line *lp*[8] (*l* being the intersection of *zv* with the zone-line [100:001] and *p*, the intersection of a line thru *z* parallel to the zone-line [100:001] with the circle of projection). A line through *x* parallel to *lzv* gives *w*. Then *zw* equals *c* in terms of the radius. A line *zn* through *z* normal to the zone-line [001:011] gives the point *n* on the zone-line [101:111]. An arc with the radius *un* gives the point *y* on the line *uhy*. Then *yz* is equal to c/a in terms of the radius. In order to determine *a*, the distance *zr* equal to *zw* is laid off on the line *zy*. Then draw any radius such as *zt*. Connect *y* and *t* and from the point *r* draw *rq* parallel to *yt*. Then *zq* equals *a* in terms of the radius of the circle. Graphically determined values for *a* and *c* are respectively 0.728 and 0.900 which check well with the calculated values.

The graphic method just outlined was described by the writer.[9]

Since the closely related mineral amarantite is also triclinic, the question arises as to whether the Knoxville crystals are not amar-

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[8] To avoid confusion *lp* is not drawn.

[9] *School of Mines Quarterly*, vol. **29**, pp. 28–29, 1907.

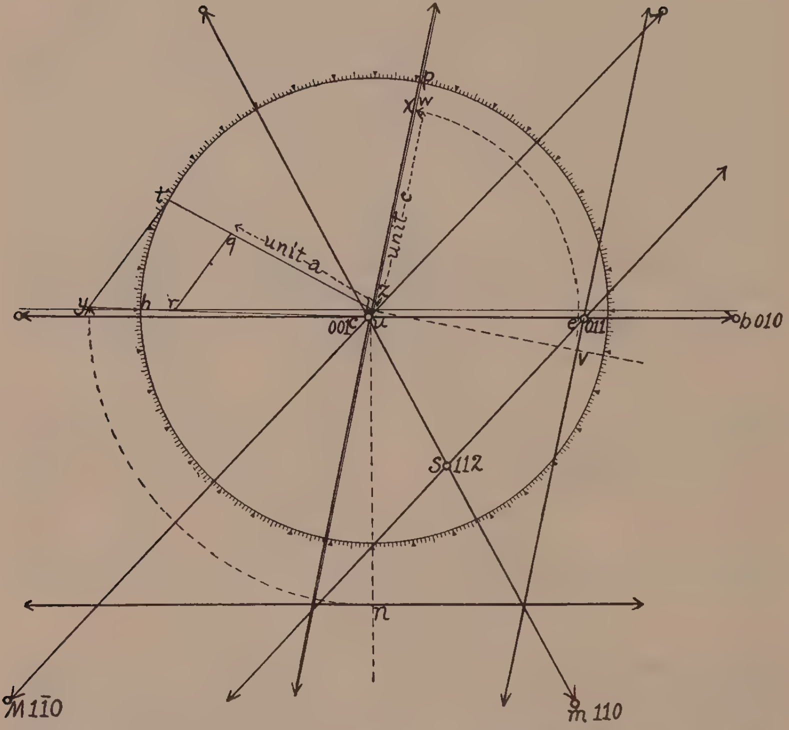

Fig. 4. Gnomonic projection of castanite showing graphic determination of the axial ratio $a:b:c$.

antite with a different orientation than that given by Penfield.[10] Although two of the interfacial angles for amarantite (100 $\wedge$ 001 = 88° 53′ and 001 $\wedge$ 111 = 42° 46′) are close to two for castanite (100 $\wedge$ 001 = 88° 48′ and 001 $\wedge$ 011 = 42° 32′) the other angles do not check. As far as I can judge from the geometrical crystallography, castanite and amarantite are different minerals. It is fortunate that the one-circle measurements of Penfield are available, for with the data given in Goldschmidt's Winkeltabellen it would be difficult to prove that castanite is a distinctive mineral. Two-circle measurements have some serious limitations.

In case more complex crystals of castanite are found in the future it may be convenient to have a list of coördinate angles available. And so coördinate angles for the known forms of castanite have been calculated by the formulae for transforming interfacial angles to coördinate angles given by Moses and Rogers.[11] The following are the angles obtained:

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[10] *Am. Jour. Sci.*, [3], vol. **40**, p. 199, 1890.

COÖRDINATE ANGLES FOR CASTANITE

	ϕ	ρ
(001)	108°55′	1°14′
(011)	1 17	42 9
(112)	62 56	33 8
(010)	0 0	90 0
(100)	101 14	90 0
(110)	61 34	90 0
(1$\bar{1}$0)	133 11	90 0

For the three first forms good graphic checks were obtained as follows: ϕ^{001}(109° 10′), ρ^{001}(1° 15′), ϕ^{011}(1° 30′), ρ^{011}(42° 12′), ϕ^{112}(63° 40′) ρ^{112}(35° 30′). The polar elements and symbols of Goldschmidt are not used, for in the opinion of the writer they serve no useful purpose.

CLEAVAGE

There is perfect cleavage parallel to (010) and less perfect parallel to (110) and (1$\bar{1}$0).

OPTICAL CRYSTALLOGRAPHY

Cleavage flakes parallel to (010) give a brownish-red color for vibrations parallel to the slower ray and a medium yellow for vibrations parallel to the faster ray. The faster ray makes an angle of about 22° with the trace of the *c*-axis. The sketch of Fig. 5 gives an idea of the behavior of the cleavage fragments in polarized light. With convergent light a somewhat eccentric biaxial interference figure with moderate 2V and high dispersion is obtained. Besides being eccentric the axial plane is somewhat inclined to (010) as shown in Fig. 6. The optical character is negative.

The principal indices of refraction are: $n_\alpha = 1.553 \pm .003$, $n_\beta = 1.643 \pm .003$, $n_\gamma = 1.657 \pm .003$; $n_\gamma - n_\alpha = 0.104 \pm .006$. These values were found by the immersion method.

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[11] *School of Mines Quarterly*, vol. **24**, p. 36, 1902; also *Zeit. f. Kryst. u. Min.*, vol. **38**, p. 226, 1903.

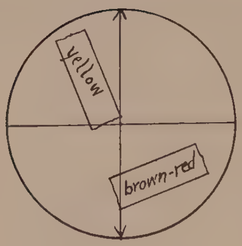

Fig. 5.

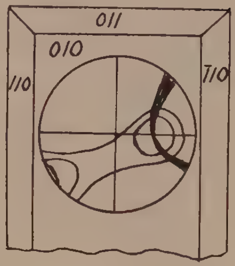

Fig. 6.

Fig. 5. Cleavage flakes of castanite in polarized light.
Fig. 6. Interference figure of castanite on (010).

Specific Gravity

The specific gravity of the castanite is about 2.2 as judged by its behavior in a mixture of methylene iodide and benzol.

Pyrognostic Tests

Heated in the closed tube the castanite turns dark and gives water which has an acid reaction.

Carefully heated before the blowpipe in platinum forceps, a fragment of the mineral turns first pale orange, then grayish brown, next dark red, and finally black, and becomes rounded on the edges (fusibility about 5). If a long splinter is heated at the extreme tip the various colors mentioned may be observed on the splinter as shown in the sketch of Fig. 7 with the original brown at the lower unheated end.

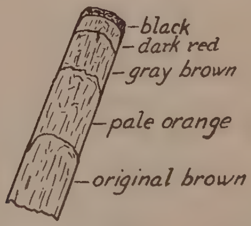

Fig. 7. Heated splinter of castanite (×10).

Chemical Properties

The castanite is practically insoluble in cold water, but it is decomposed by hot water. It is easily soluble in hydrochloric acid and the solution gives tests for ferric iron and the sulfate radical. All the iron is in the ferric condition and no aluminum and only a trace of magnesium is present.

A chemical analysis made by my colleague, Mr. O. C. Shepard, furnished the following results:

ANALYSIS OF CASTANITE BY O. C. SHEPARD

		Mol. Ratios		Theory
Fe_2O_3	34.47	0.215	1	34.58
SO_3	35.11	0.438	2.03	34.58
$H_2O+110°C=14.58$ $H_2O-110°C=15.73$	30.31	1.685	7.83	30.84
Insol.	0.22			
Total	100.21			

The molecular ratios are 1:2.03:7.83, which is very close to the empirical formula $Fe_2O_3 \cdot 2SO_3 \cdot 8H_2O$ assigned to castanite by Darapsky.

Castanite is stable at ordinary room temperature, but specimens on a window sill exposed to the sun changed from burnt orange to pale orange and gradually fell to a powder. Several specimens were spoiled in this way.

Dehydration tests were carried out by Mr. Shepard at varying temperatures. The only prominent break is at 27°C. Heated for nine days at this temperature the loss in weight is 14.91 per cent (average of 14.83 and 14.98 for two samples of different weights).

This indicates that the composition for the compound formed is $Fe_2O_3 \cdot 2SO_3 \cdot 4H_2O$. On changing from $Fe_2O_3 \cdot 2SO_3 \cdot 8H_2O$ to $Fe_2O_3 \cdot 2SO_3 \cdot 4H_2O$ the loss in weight should be 15.57 per cent. A mineral with the composition $Fe_2O_3 \cdot 2SO_3 \cdot 4H_2O$ from Chile was analyzed by Mackintosh[12] but the mineral was not named or adequately described although it was stated that it was perhaps an alteration of amarantite. At 100°C the loss in weight is only 15.62 per cent. Had sufficient time been given, the loss would probably have been attained at 27°C. Heated at intervals of 20°C the loss in weight is gradual until a temperature of 360°C is reached, when the loss is 30.97 per cent which is the total water content (theoretical amount =30.84 per cent).

COMPOUNDS OF THE $Fe_2O_3 \cdot 2SO_3 \cdot nH_2O$ SERIES

In addition to castanite there are a number of other compounds of the $Fe_2O_3 \cdot 2SO_3 \cdot nH_2O$ series with the variations in the value of n. The following have come under my notice:

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[12] *Am. Jour. Sci.* [3], vol. **38**, p. 243–5, 1889.

$Fe_2O_3 \cdot 2SO_3 \cdot H_2O$	( )	Orthorhombic.	Maus, 1827.
$Fe_2O_3 \cdot 2SO_3 \cdot 3H_2O$	(Rubrite)	?	Darapsky, 1890.
$Fe_2O_3 \cdot 2SO_3 \cdot 4H_2O$	( )	?	Mackintosh, 1889.
$Fe_2O_3 \cdot 2SO_3 \cdot 5H_2O$	(Butlerite?)	Monoclinic.	Posnjak and Merwin, 1922.
$Fe_2O_3 \cdot 2SO_3 \cdot 7H_2O$	(Amarantite)	Triclinic.	Frenzel, 1887.
$Fe_2O_3 \cdot 2SO_3 \cdot 8H_2O$	(Castanite)	Triclinic.	Darapsky, 1890.
$Fe_2O_3 \cdot 2SO_3 \cdot 10H_2O$	(Fibroferrite)	Monoclinic?	Rose, 1833.

This is a remarkable series of hydrates, but they are not all well-established. Posnjak and Merwin[13] in a rather elaborate study of the Fe_2O_3-SO_3-H_2O system produced $Fe_2O_3 \cdot 2SO_3 \cdot H_2O$ and $Fe_2O_3 \cdot 2SO_3 \cdot 5H_2O$ within the temperature range of 50°–200°C. What is possibly a dimorphous form of $Fe_2O_3 \cdot 2SO_3 \cdot 5H_2O$ was described under the name "butlerite" by Lausen.[14] They failed to obtain $Fe_2O_3 \cdot 2SO_3 \cdot 3H_2O$, the rubrite of Darapsky,[15] for which there is no adequate mineralogical description. As a consequence it has not been accepted as a mineral. They also failed to produce $Fe_2O_3 \cdot 2SO_3 \cdot 4H_2O$, which was assigned to an unnamed mineral from Chile by Mackintosh. There is no adequate description of this compound and its status is doubtful.

The amarantite, castanite, and fibroferrite are now well-established minerals and the failure of Posnjak and Merwin to obtain these minerals is due to the fact that they worked above 50°C.

ORIGIN OF THE CASTANITE

That castanite is a low-temperature mineral seems certain because it is unstable above 27°C and because Posnjak and Merwin failed to produce it at temperatures above 50°C. In view of its close association with sulfur and cinnabar it seems likely that castanite is a low-temperature solfataric mineral. Its ultimate source is in all probability the marcasite and pyrite which are prominent in some parts of the mine.

VALIDITY OF CASTANITE

The crystallographic study combined with the chemical analysis indicates that castanite is a definite mineral with the formula $Fe_2O_3 \cdot 2SO_3 \cdot 8H_2O$.

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[13] *Jour. Am. Chem. Soc.*, vol. **44**, pp. 1965–94, 1922.

[14] This journal, vol. **13**, p. 211, 1928.

[15] *N. Jb. f. Min.*, **1890**, 1, p. 65.

NOTES AND NEWS

FRANK WIGGLESWORTH CLARKE

Frank Wigglesworth Clarke died at his residence in Washington, D. C., on May 23, 1931, two months after he passed his eighty-fourth year. Retired from Government service on January 1, 1925, he had been Chief Chemist of the U. S. Geological Survey for a long span of time, having been appointed in 1883. During the same time he was honorary Curator of minerals in the United States National Museum but he took a much more active interest in his curatorship than would be inferred from that title, and the excellence and comprehensiveness of the mineral collection in the Museum are due in large measure to this active interest and to his painstaking efforts both in the collection and exhibition of specimens.

Frank W. Clarke, 1847–1931

The holder of many degrees and titles, he was known by his co-workers as "The Professor," a title inherited from his professorships at Howard University 1873–74, and at the University of Cincinnati 1874–83.

While primarily a chemist, his second love was for minerals, naturally along chemical lines. His first paper, published in 1868, several days before he was 21, bears the title: "On a new process in mineral analysis." His bibliography of over 300 papers covers a wide range of subjects from abstruse theoretical deductions (he was the first to present a consistent theory of the evolution of the chemical elements) to poetry.

Possessor of a remarkably retentive memory, with ready command of all his accumulated information, Prof. Clarke never seemed able, as his 60 year long friend, Charles E. Munroe, has said, "to recall any but pleasant things of those of whom he speaks. . . . I have never known him to say a disagreeable thing of any person."

That wonderful compendium, "Data of Geochemistry," in its fifth edition, bears eloquent testimony to his natural ability to consider fully and appreciatively the views of others, at times not in accord with his own views, and to present what seemed to him to be the truest interpretation of the many natural phenomena in which he was so keenly interested, in a way that could give offense to none.

He was among the first to compile fundamental physical and chemical constants and his "Constants of Nature," published by the Smithsonian Institution in 1876, and his many papers on "Atomic Weights," were long standards of reference.

His connection with the Geological Survey in 1883 gave a definite stimulus to his mineralogical interests and thenceforward he contributed a steady stream of papers and larger reports on mineralogy and on what may be called chemical geology. In the analysis of a mineral he was never satisfied with only the analytical results but always wanted to know the associations, the alterations, and the syntheses of the mineral.

He tried to express the composition of minerals by a coordination of known facts so as to show their constitution, their structure, and their relations to other minerals. He began with the silicates as they are by far the most important constituents of the solid crust of the earth and published his first "Constitution of the silicates" in 1895. Clarke was always greatly interested in what he called the natural history of a mineral, especially its alteration products and pseudomorphs, for to him the alteration products were the records of chemical changes. No less important to him were the laboratory syntheses and artificial transformations which could be carried out experimentally. All these reactions afforded information as to the constitution of minerals. As he has said: "A good formula indicates the convergence of knowledge; if it fulfills that purpose it is useful, even though it may be supplanted at some later day by an expression of still greater generality."

A compiler par excellence one nevertheless wonders how he found time in addition to his administrative work, reports on atomic weights, chemical and physical data, and numerous shorter papers, to compile such more lengthy reports as "Analyses of rocks and minerals," "Water analyses," "Data of Geochemistry," "Inorganic Constituents of Marine Invertebrates," "The Composition of the Earth's Crust," "The Composition of the River and Lake Waters"—all published by the U. S. Geological Survey.

Several times in the past, at the suggestion that his name be given to a new mineral, he had modestly suggested other names which he considered more appropriate. However, the description of "Clarkeite, a New Uranium Mineral," appeared about a week before his death.

The lighter side of life always appealed to him. A guest at a Thanksgiving dinner, when the host had difficulty in carving the turkey, Clarke suggested that it might profit the carver to visit the National Museum, for a certain door therein bears on it the sign Division of Birds.

As one of the many who have served under him, the writer feels the loss keenly. Always kind and generous and very free of his immense store of knowledge, it was indeed a privilege to have been associated with and to have worked under the direction of so able a Chief Chemist.

W. T. SCHALLER

Dr. Arthur S. Eakle, professor emeritus of mineralogy at the University of California died in Honolulu July 5, after a brief illness. Professor Eakle was a former president of the Mineralogical Society of America and at the time of his death was actively engaged in making a mineral survey of the Hawaiian Islands.

Albert C. Burrage, a member of the Mineralogical Society of America, died at his summer home in West Manchester, Mass., June 29 at the age of 71. His interests were numerous and varied. Mr. Burrage was one of the organizers of the Amalgamated Copper Company and was largely responsible for the development of the Chilean copper deposits.

Albert C. Bates, an enthusiastic member of the Newark Mineralogical Society, died at his home on May 5 in the 75th year of his age. He was especially interested in collecting and examining crystals of quartz.

Mr. Rudolph G. Sohlberg of the University of Michigan has been appointed Teaching Fellow in Mineralogy at Stanford University.

PROCEEDINGS OF SOCIETIES

MINERALOGICAL SOCIETY OF GREAT BRITAIN AND IRELAND

Mineralogical Society, *June 9*.—Sir John S. Flett, President, in the chair.

Mr. G. E. L. Carter: *On an occurrence of vanadiferous nodules on the coast of South Devon.* The author describes an occurrence of vanadiferous nodules in the red marls that underlie the Budleigh Salterton pebble beds on the coast of South Devon. These nodules consist of siliceous and argillaceous material impregnated with vanadium oxide and calcium carbonate. A typical nodule examined at the Imperial Institute showed a roughly concentric structure, ill-defined black shells alternating with shells of light-coloured material. Radiating black bands stood out as ribs on the surface of the nodule. Analyses by Miss Hilda Bennett showed that the black portion of the nodule contained 13.96 per cent of vanadium oxide, estimated as pentoxide. The light-coloured portion of the nodule contained only 1.91 per cent of vanadium oxide, and was relatively richer in calcareous and siliceous matter than the blacker and more vanadiferous portion. The occurrence deserves investigation from the economic point of view, as vanadium minerals are of sparse distribution. A preliminary optical and *X*-ray examination by Mr. F. A. Bannister of the darker material of the nodules suggests the presence of a vanadiferous chlorite.

Mr. Max H. Hey: *Studies on the Zeolites. Part II.* Thomsonite (including faroelite) and gonnardite. An analytical, optical and *X*-ray study of a considerable number of thomsonite specimens has led to the conclusion that thomsonite and faroelite form a continuous isomorphous series. The true symmetry of thomsonite is shown to be didigonal polar (C_{2v}). The unit cell is shown to contain $(Ca, Na)_6 (Al, Si)_{20}O_{40} \cdot 12H_2O$. The mean refractive index ranges from 1.517 to 1.535, falling with increase in the Si/Al ratio. Apparatus has been designed and applied to measure the vapour pressure of thomsonite at various temperatures and degrees of dehydration, and it appears very probable that a dimorphous high-temperature form exists, the transition being readily reversible. Gonnardite is probably identical with the high temperature dimorphous form of thomsonite (meta-thomsonite) and is therefore to be regarded as a separate species.

Mr. Arthur Russell: *An account of British Mineral collectors and dealers in the 17th, 18th and 19th centuries.* A second installment:—John Woodward (1665–1728), and Charles Francis Greville (1749–1809).

Dr. L. J. Spencer: *Hoba (South-West Africa), the largest known meteorite.* The large mass of meteoric iron discovered in 1920 on Hoba West farm, 12 miles west of Grootfontein measures about 10 x 9 feet on its flat upper surface, and is estimated to weigh 60 metric tons. It belongs to the group of nickel-rich ataxites. Chemical analysis by Mr. H. H. Hey shows: Fe 83.44, Ni 16.24 per cent, with small amounts of cobalt, copper, sulphur, phosphorus, and carbon. Photomicrographs (×820) by Dr. J. M. Robertson show a minute plessite-like structure.

Dr. L. J. Spencer: *Twelfth List of new mineral names.* Since the publication in 1928 of the eleventh list of this series (the first was in 1897) 120 names have been collected from the current literature. In addition to the bibliographical reference, a brief description of the essential characters of the mineral and derivation of the name are given.

DR. J. DRUGMAN: *On different habits of fluorite crystals.* In fluorite the cube is usually the predominating form. Crystals of other habits—octahedral, rhombic-dodecahedral, and triakis-octahedral—are described. The temperature during the growth of the crystal has perhaps influenced its habit.

BOOK REVIEW

THE WORKING OF SEMI-PRECIOUS STONES, J. H. HOWARD. 37 pages, 12 figures, and 18 plates. Rocks and Minerals, Peekskill, N. Y. $1.00.

This little booklet should furnish collectors with the inspiration for cutting and polishing some of our more common gem minerals. The author, an amateur lapidary, presents in detail the method used for cutting and polishing cabochon surfaces in such a simple and direct manner that one is convinced that the art is not so difficult as to be beyond the ability of the ordinary layman. One chapter is devoted to faceted cuts and another to the sawing of minerals. Complete directions are given for the construction of the necessary apparatus, the cost of which the author states should not exceed $45.00.

C. B. SLAWSON

NEW MINERAL NAMES

Nicolayite

NAME: In honor of Rev. C. G. Nicolay, early mineral collector in Western Australia. Formerly called thorogummite.

CHEMICAL PROPERTIES: A hydrous silicate of lead, thorium and uranium, differing from maitlandite in the state of oxidation of the uranium, $2(Pb, Ca)O \cdot 3ThO_2 \cdot 4UO_3 \cdot 8SiO_2 \cdot 21H_2O$. Analysis: UO_3 37.33, UO_2 *nil*, ThO_2 24.46, SiO_2 15.30, Ce_2O_3 .12, Yt_2O_3 .32, PbO 7.78, MnO *nil*, CaO 1.62, MgO .16, H_2O+8.37, H_2O- 4.19, $(Ta, Cb)_2O_5$ .40; total 100.05.

PHYSICAL AND OPTICAL PROPERTIES: Color yellow, luster vitreous. Amorphous. $n=1.617$. $G=4.13$.

OCCURRENCE: Like maitlandite.

W. F. FOSHAG

Montasite

H. L. KIRKMAN: Some notes on Crocidolite and Amosite Occurrences in the Union. *Trans. Geol. Soc. S. Africa*, **33**, 17, 1931.

A registered name for asbestos fiber from the Montana mine, Pietersburg-Lydenburg district, South Africa.

W. F. F.

NEW DATA

Cooperite

H. R. Adams: Notes on Platinum Minerals from Rustenburg and Potgietersrust District, Transvaal. *Trans. Geol. Soc. S. Africa,* **33,** 103–110, 1931. *Cf. Am. Mineral.,* **14,** 339, 1929.

Chemical Properties: A sulfide of platinum, PtS_2. Analyses: (Potgietersrust) Pt 71.5, Pd 6.4, S 14.1, As 3.4, Ni 2.0, insol. 1.5; (Rustenburg) Pt 72.9, Pd 6.2, S 15.0, As 0.2, Ni 2.2, insol. 2.6. Relatively insoluble in aqua regia.

Crystallographic Properties: Orthorhombic. Habit prismatic. $a:b:c=0.4968:1:2.0025$. Forms $c(001)$, $b(010)$, $a(100)$, $e(101)$, $f(201)$, $g(221)$. Twinning polysynthetically (?) parallel to (010).

Physical Properties: Color silver white with yellowish tinge. Luster metallic. Cleavage none. Fracture conchoidal, very brittle. Magnetic susceptibility weak. Hd. 5.5. G. 9.0.

Mineralographic Properties: Practically unaffected by etching reagents. On heating at 800°–900°C for a few seconds particles become colored blue and bronze by oxidation films. Examinations of particles, especially those from Potgietersrust often reveals two constituents, the main one being a darker sulfide, the other (probably sperrylite) having a microcrystalline and more silvery appearance.

W. F. F.